ISBN : 978-93-6342-558-3

दयानंद शिक्षण संस्था,लातूर

आ नो भद्राः क्रतवो यन्तु विश्वतः

Dayanand Education Society's

Dayanand Science College, Latur

Affiliated to Swami Ramanand Teerth Marathwada University,
Nanded, Maharashtra, India

Conference Proceeding

International Conference on Chemistry for Society, Health, Industries and Pharmacy (ICCSHIP-2025)

12th to 15th February 2025

Organized by

Department of Chemistry, Dayanand Science College, Latur
Maharashtra, India

Welcome to Latur……

Dear Esteemed Participants,

The city is located in India's Maharashtra State's Marathwada area. It serves as Latur District's headquarters. Surrounded by numerous historical landmarks, it is a popular tourist destination. In Maharashtra State, Latur is a renowned center for high-quality education.

y road and rail from the international airport in Mumbai, and 298 kilometers by road and rail from the international airport in Hyderabad. Latur is located 280 kilometers from Aurangabad, the closest domestic airport. Latur has a number of tourist attractions including the Udgir Fort (50km), Naldurga Fort (80Km), which played a significant role in the battle between the Marathas and the Nizam's army.

About the Institution

Dayanand Education Society is one of the oldest educational Institutions which were established in 1961. The motto of institute is **"Let the noble thoughts come to us from all the directions of the universe".** In the campus of Dayanand Education Institute there are eight different Colleges imparting education from Junior to Senior College level to 18,500 students. In this Institute, about 960 teaching and non-teaching staff who constantly strives hard to achieves the mission and goals of the Society.

About the College,

Dayanand Science College, Latur, is unique, first oldest and the finest single faculty college in the region of Marathwada, pursuing excellence in science education with several branches. Due to the quality education, the college received different National and International awards and schemes. The College has **13** subject combinations for UG programs, **08** PG programs, **05** Research centres and **28** COP/Value added courses. The Research centres have collaboration with the other scientific Institution research centres and scientists of the various countries, such as USA, Korea, Switzerland, Poland, Greece, Malaysia, Romania, Oman, Thailand and Singapore etc. In last five years college organized 06 Inspire science campus, 4 national level refresher courses, 3 International, 18 National, 12 State/ Regional conferences and workshops. In the year 2022, College had been awarded **"A+"** grade in **NAAC Accreditation 3rd cycle with CGPA 3.40.** Recently college has achieved First Prize in **National Energy Conservation Award - 2022** given by Ministry of Power, Bureau of Energy Efficiency of Govt. of India on 14th December 2022. In the year 2015 College received "**Best College (Urban) Award"** from S.R.T.M. University, Nanded college was granted the "**College with Potential for Excellence Award (CPE)**" by the UGC in 2016 and was granted a grant of Rs. 5 crores in three stages. In 2018, the college has obtained a Rs 2 Cr **Rusa Infrastructure grant**. The MGNCRE under MHRD presented the college with the "**One District One Green Champion**" award for campus environment. Additionally, Microsoft India recognized the college as an Innovative College in the teaching of digital technologies. The college has extensive knowledge of the evolution of the "**Latur Pattern of Education**" in Maharashtra due to its meritorious nature.

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ICCSHIP-2025

International Conference on Chemistry for Society, Health, Industries & Pharmacy
February, 12-15,2025

Abstracts/ Conference Proceedings Book

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Principal
Dayanand Science College, Latur (Chairman)

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- **Dr. N. A. Kedar**
- **Dr. J. A. Angulwar**
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ABOUT DAYANAND SCIENCE COLLEGE

Dayanand Science College, Latur, is unique, first oldest and the finest single faculty college in the region of Marathwada, pursuing excellence in science education with several branches. Due to the quality education, the college received different National and International awards and schemes. The College has **13** subject combinations for UG programs, **08** PG programs, **05** Research centres and **28** COP/Value added courses. The Research centres have collaboration with the other scientific Institution research centres and scientists of the various countries, such as USA, Korea, Switzerland, Poland, Greece, Malaysia, Romania, Oman, Thailand and Singapore etc. In last five years college organized 06 Inspire science camp, 4 national level refresher courses, 3 International, 18 National, 12 State/ Regional conferences and workshops. In the year 2022, College has been awarded **"A^+"** grade in **NAAC Accreditation 3rd cycle with CGPA 3.40.** Recently college has achieved First Prize in **National Energy Conservation Award - 2022** given by Ministry of Power, Bureau of Energy Efficiency of Govt. of India on 14th December 2022. In the year 2015 College received "**Best College (Urban) Award" from S.R.T.M. University, Nanded** college was granted the "**College with Potential for Excellence Award (CPE)**" by the UGC in 2016 and was granted a grant of Rs. 5 crores in three stages. In 2018, the college has obtained a **Rs 2 Cr RUSA Infrastructure grant**. The MGNCRE under MHRD presented the college with the "**One District One Green Champion**" award for campus environment. Additionally, Microsoft India recognized the college as an Innovative College in the teaching of digital technologies. The college has extensive knowledge of the evolution of the "**Latur Pattern of Education**" in Maharashtra due to its meritorious nature.

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: Vision:

To enlight of rural and contribute their service for universal development by promoting education

: Mission Statement:

आ नो भद्राः क्रतवो यन्तु विश्वतः

Let the noble thoughts come to us from all the directions of the universe

: Goals and Objectives:

- To provide quality academic environment for effective teaching, learning and research in basic sciences.
- To develop a scientific temperament through a strong academic foundation coupled with practical exercises.
- To impart higher education in science to the students of our rural area of this region.
- To promote the activities that are necessary for the welfare and overall development.
- To help needy and economically weaker students in education.
- To prepare the students to face the challenges of the competitive world.
- To inculcate discipline sincerity and devotion among the students to make them most responsible and respectable citizens of India.
- To motivate students for acquiring scientific skills and creativity.
- To collaborate with stakeholders of higher education for quality signs education and research.
- To create socio-environmental awareness among students and masses around.
- To build multi-dimensional personality of students.

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978-93-6342-558-3

MESSAGE

सी. पी. राधाकृष्णन
C. P. Radhakrishnan

सत्यमेव जयते

राज भवन,
मलबार हिल, मुंबई ४०० ०३५
RAJ BHAVAN,
Malabar Hill, Mumbai 400 035

29 January 2025

राज्यपाल, महाराष्ट्र
GOVERNOR OF MAHARASHTRA

MESSAGE

I am pleased to know that the Dayanand Education Society's Dayanand Science College, Latur is organising an International Conference on Chemistry for Society, Health, Industry and Pharmacy (ICCSHIP-2025) at Latur from 12th to 15th February 2025.

I congratulate the Dayanand Science College for organizing the Conference and wish the participants fruitful delibration.

(C. P. Radhakrishnan)

ISBN NO.:
978-93-6342-558-3

MINISTER
HIGHER AND TECHNICAL EDUCATION, PARLIAMENTARY AFFAIRS
MAHARASHTRA STATE
Mantralaya, Mumbai 400 032
cbpatil.minister@gmail.com

Date : 29 JAN 2025

:: MESSAGE ::

On behalf of the Ministry of Higher Education, Government of Maharashtra, I extend my warm greetings and a heartfelt welcome to the International Conference on Chemistry for Society, Health, Industry, and Pharmacy, Organized by the Department of Chemistry at Dayanand Science College, Latur, This esteemed conference brings together experts from across the globe to exchange knowledge, ideas, and innovations in chemistry with a particular focus on its applications in society, healthcare industry and pharmacy.

Maharashtra has a proud legacy of academic excellence, and we remain committed to fostering a culture of research, innovation and interdisciplinary collaboration. This conference aligns with our vision of advancing scientific progress and addressing global challenges through meaningful discourse and knowledge-sharing. I commend the Department of Chemistry at Dayanand Science College, Latur, for their dedication and efforts in organizing this prestigious event. I encourage all participants to actively engage in discussions, share their insights, and explore opportunities for collaboration.

Thank you for being a part of this conference. I wish you a productive, insightful and enriching experience.

With warm Regards.

C. B. Patil

(Chandrakant (Dada) Patil)

ISBN NO.:
978-93-6342-558-3

Government of Maharashtra

D.O.No. 01/2025/ACS/HTED
Higher & Technical Education Department
Mantralaya, Mumbai

Date: 29th January, 2025

Message

It gives me immense pleasure to extend my warm greetings to the organizers, participants, and esteemed guests of the International Conference on "Chemistry in Society, Industry, and Pharmacy 2025," being organized by the Department of Chemistry, Dayanand Science College, Latur.

This conference, with its focus on the multifaceted role of chemistry in addressing societal needs, industrial advancement, and pharmaceutical innovations, provides a remarkable platform for academicians, researchers, and industry experts to collaborate, share knowledge, and explore groundbreaking solutions for global challenges.

I commend the efforts of the Department of Chemistry and the organizers for bringing together distinguished scientists and professionals from across the globe.

Chemistry plays a pivotal role in improving the quality of life by contributing to advancements in healthcare, sustainable industrial practices, and environmental protection. This conference is a timely initiative to explore cutting-edge developments, exchange ideas, and build partnerships that will shape the future of science and technology.

I am confident that the discussions and deliberations at this conference will not only contribute to the academic and scientific community but also inspire innovative solutions to address the pressing needs of society.

My best wishes to all the participants for a fruitful and intellectually enriching experience. May this conference pave the way for new ideas and collaborations that advance the frontiers of science and serve humanity.

With best compliments,

(B. Venugopal Reddy)

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Dr. Manohar G. Chaskar
M.Sc. Ph.D., Mombushuo Fellow (Japan)
VICE-CHANCELLOR
डॉ. मनोहर ग. चासकर
एम्. एस्सी., पीएच्.डी., मॉम्बुशो फेलो (जपान)
कुलगुरु

SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY
NANDED – 431 606 (Maharashtra)
स्वामी रामानंद तीर्थ मराठवाडा विद्यापीठ
नांदेड – ४३१ ६०६ (महाराष्ट्र)

Established by Govt. of Maharashtra on 17th September 1994, Recognized by the UGC U/s 2(f) and 12(B), NAAC Re-accredited with B++ Grade, a State University

SRTMUN/VC_Message/2024-25/129 February 05, 2025

VICE-CHANCELLOR'S MESSAGE

I am very happy to know that Dayanand Education Society's Dayanand Science College, Latur, Maharashtra State, India is organizing a International Conference (offline) on "Chemistry for Society, Health, Industry and Pharmacy (ICCSHIP-2025)" to be held during 13-15th February, 2025.

We appreciate your tireless efforts in hosting the International Conference on Chemistry for Society, Health, Industries & Pharmacy (ICCSHIP-2025). Your dedication to fostering a platform for knowledge sharing, collaboration, and innovation in chemistry is commendable. We wish you continued success in bringing together renowned experts, researchers, and scholars from around the world. Your contributions will significantly impact the advancement of chemical sciences and its applications.

I wish the organizers a grand success of the International conference. I also extend my best wishes to all participants and contributors of the conference.

"I think the girl can do anything! She just needs to believe in herself."

(Manohar Chaskar)
Vice-Chancellor

To
Principal,
Dayanand Science College,
Barshi Rd, Prakash Nagar,
Latur - 413 531.

"Dnyanteerth", Vishnupuri NANDED – 431 606 (Maharashtra), India
Ph: (+91-2462) (O) 215282, Telefax : 215245
Website : www.srtmun.ac.in, E-Mail : vcoffice@srtmun.ac.in

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Punyashlok Ahilyadevi Holkar
Solapur University, Solapur
Kegaon, Solapur - 413 255, Maharashtra (India)

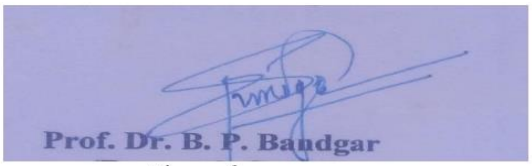
Dear Esteemed Participants,

I am very happy because Dayanand Science College, Latur is going to organize International Conference on Chemistry in Society, Health, Industry and Pharmacy on 12-15 February 2025. I am delighted to extend my warmest greetings to the organizers, participants, and attendees of the International Conference on Chemistry for Society, Health, Industry, and Pharmacy (ICCSHIP-2025).

As a former Vice-Chancellor of Solapur University, I have witnessed first-hand the transformative power of chemistry in addressing societal challenges. ICCSHIP-2025 provides a unique platform for global experts to converge, share knowledge, and foster collaborations that can drive innovation and sustainable development.

I commend the organizers for their tireless efforts in bringing together such a diverse and esteemed group of speakers and participants. I am confident that ICCSHIP-2025 will be a resounding success, paving the way for new discoveries, breakthroughs, and applications of chemistry in various fields. I wish you all a productive, engaging, and enriching experience at ICCSHIP-2025. Thank you for your participation.

Best regards.



Sincerely,
Prof. B. P. Bandgar
Former Vice-Chancellor, Punyashlok Ahilyadevi Holkar Solapur University, Solapur

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(Reg. no. F- 13 Latur)

"आ नो भद्राः कृतवो यन्तु विश्वतः"

Dayanand Education Society, Latur.

Ref. No.: Date : 06.01.2025

MESSAGE

I am glad to know that, the Department of Chemistry, Dayanand Science College, Latur is organizing the International Conference on " Chemistry for Society, Health, Industry and Pharmacy" (ICCSHIP-2025)," during February 12-15, 2025 at Department of Chemistry under the sponsorship of Dayanand Education Society and University Grant Commission.

I am sure that this International Conference will provide a forum to the academicians and researchers to share their views and disseminate the useful research findings and innovative thoughts on "Chemistry for Society, Health, Industry and Pharmacy". The chemistry and perspective of this conference will be fruitful in providing ways and means to expand the initiatives giving valuable insight to the participants.

I congratulate Dr. S. S. Bellale, Principal and his team for organizing the International Conference on "Chemistry for Society, Health, Industry and Pharmacy". I convey my best wishes for the success of the conference.

Laxmiraman Lahoti,
President,
Dayanand Education Society,
Latur.

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(Reg. no. F- 13 Latur)

"आ नो भद्राः कृतवो यन्तु विश्वतः"

Dayanand Education Society, Latur.

Ref. No.: Date : 06.01.2025

MESSAGE

My belief in the creation of a miraculous universe is totally based on Chemistry, the role of chemistry in the very existence of life on earth plays a great value.

I am glad that the International Conference of Chemistry is taking place in our institution. I welcome scholars from abroad and across India to this conference. The staff of this College has always been trying for excellence. I wish them and the event every success.

I hope this conference proves to be the first step towards a full-fledged approach for interaction among Chemists. I appreciate the initiatives of the Institute in this regard and I am sure, such efforts would go a long way in creating research based activities in chemistry for present and future generations. I congratulate Principal Dr. S. S. Bellale, Organizing Secretary Dr. R. S. Shinde, Convener Dr. N.A. Kedar, all professors, students who are directly and indirectly involved in this conference for the success.

Arvind Sonvane,
(B.E. Civil Honors),
Vice-President,
Dayanand Education Society,
Latur.

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(Reg. no. F- 13 Latur)

Dayanand Education Society, Latur.

Ref. No.:

Date : 18-01-2025

MESSAGE

I am glad to know that the Department of Chemistry, Dayanand Science College, Latur is organizing the International Conference on "Chemistry for Society, Health, Industry and Pharmacy" (ICCSHIP-2025)," during February 12-15, 2025.

This conference will provide a useful platform for all the participants including students, research scholars, academicians and scientists to interact, discuss and enrich latest developing areas in applied chemistry.

I appreciate the efforts made by the Chairman, Organizing Secretary, Convener and other teaching staff for organizing this Seminar. I offer my best wishes for effective and successful conduct of this seminar.

Ramesh Biyani,
Secretary,
Dayanand Education Society,
Latur.

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NAAC 3rd Cycle : A+ (CGPA 3.40)
DST-FIST (Recognition)
UGC-CPE (Status)
National 1st Prize NECA (GOI)
Best College Award (STRMUN)

Establishment : June 1961
AISHE: C-7327; College Code: 303
Ph.No. : (02382) 221149, 222929
Web. : www.dsclatur.org
E-mail : daya_scin1@rediffmail.com

Dayanand Education Society's
Dayanand Science College, Latur
Maharashtra, India
(Affiliated to Swami Ramanand Teerth Marathwada University, Nanded)

Laxmiraman Lahoti
President

Ramesh Biyani
Secretary

Dr. Sidheshwar Bellale
I/c Principal

Date : 28-01-2025

MESSAGE

It gives me an immense pleasure to welcome you to the four day International Conference on **"Chemistry for Society, Health, Industry and Pharmacy" (ICCSHIP-2025)** during February 12-15, 2025. I take this opportunity to congratulate Dr. R. S. Shinde and Dr. N. A. Kedar for organizing this event in our Institute.

Chemistry is significant in our civilization because it affects our basic needs for food, clothing, shelter, health, energy, and clean air, water, and soil, among other things. Chemistry has contributed to the development of many industries, including, Sugar, Cement, Paper, Glass Textile, Pharmaceuticals, Paints, Pigments, Leather, Petroleum, Plastics. Chemistry has also helped to discover and develop new products, such as: Synthetic fibers, Adhesives, Cosmetics, Electronic components, Lubricants.

I am sure this conference will provide a unique opportunity for everyone for in-depth technical discussions and exchange of ideas in the new era of chemistry and applied sciences, as well as the potential of their applications in Society, Health, Pharmacy and Industries. Here we have made all the necessary arrangements for your hospitality, if any lacuna remains please bear with us. Welcome you all once again.

Thank you very much.

28.1.2025

Dr. S.S. Bellale
Principal

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Dayanand Science College, Latur
A Affiliated to Swami RamanandTeerth Marathwada University, Nanded
DEPARTMENT OF CHEMISTRY AND INDUSTRIAL CHEMISTRY
DST-FIST, NAAC Re-accredited 'A^{+}' Grade, Best college Award

Dr. Y. P. Sarnikar
Associate Professor
M.Sc. NET, B.Ed. Ph. D.
Mob. No.: +919423345365
E-mail: sarnikaryp@gmail.com
Website:www.dsclatur.org

Narayan Nagar
Ausa Road
Latur-413 512
Maharashtra (INDIA)
Phone: +91(02382)222929
Fax: +91(02382)221149

Ref: Dscl/chem./appl/01/2024-25 **Date: 03/ 02 / 2025**

Message

Dear Participants,

On behalf of the Department of Chemistry, Dayanand Science College, Latur, I warmly welcome you to the International Conference on Chemistry for Society, Health, Industry, and Pharmacy.

We are thrilled to host this prestigious event, bringing together experts from around the world to share knowledge, ideas, and innovations in chemistry. This conference provides a unique platform for you to engage with renowned speakers, share your research, and network with fellow professionals.

I am grateful to our organizers, speakers, and participants for their contributions to this event. I am confident that this conference will foster meaningful discussions, collaborations, and advancements in the field of chemistry.

Thank you for joining us, and I wish you a productive and enjoyable experience.

Sincerely,

Head, Department of Chemistry
Dayanand Science College, Latur

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Dayanand Science College, Latur
Affiliated to Swami Ramanand Teerth Marathwada University, Nanded
DEPARTMENT OF CHEMISTRY AND INDUSTRIAL CHEMISTRY
DST-FIST, NAAC Re-accredited 'A+' Grade, Best college Award

Dr. N. A. Kedar
Assistant Professor Research Supervisor
M.Sc. Ph.D.
Mob. No.: +919423350653
E-mail:nak125721@gmail.com
www.dsclatur.org

Omsteps Apartment
Ambajogai Road
Latur-413 512
Maharashtra (INDIA)
Phone: +91(02382) 222929
Fax: +91(02382)221149

Ref: Dscl/chem./ICCSHIP/02/2024-25 **Date: 25 /01 /2025**

MESSAGE

On behalf of the organizing committee, I warmly welcome you to the International Conference on Chemistry for Society, Health, Industry, and Pharmacy (ICCSHIP-2025).

We are thrilled to bring together experts from around the world to share knowledge, ideas, and innovations in chemistry. This conference provides a unique platform for you to engage with global leaders, learn about cutting-edge research, and network with fellow professionals.

Over the next few days, we will delve into the latest advancements in chemistry, exploring its applications in society, health, industry, and pharmacy. Our program features keynote addresses, technical sessions, poster presentations, and exhibitions.

I invite you to actively participate in the conference, share your insights, and contribute to the discussions. Your presence here is a testament to the importance of chemistry in addressing global challenges.

Thank you for joining us, and I wish you a productive, engaging, and enjoyable experience at ICCSHIP-2025.

Sincerely,

Dr. N. A. kedar
Convener
(ICCSHIP-2025)

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Dayanand Science College, Latur
Affiliated to Swami RamanandTeerth Marathwada University, Nanded
DEPARTMENT OF CHEMISTRY AND INDUSTRIAL CHEMISTRY
DST-FIST, NAAC Re-accredited 'A+' Grade, Best college Award

Dr. R. S. Shinde
Professor
M.Sc. SET, B.Ed. GATE, Ph. D.
Mob. No.: +919850150872
E-mail :rshinde.33381@gmail.com
Website:www.dsclatur.org

Amleshwar Nagar
Barshi Road
Latur-413 512
Maharashtra (INDIA)
Phone: +91(02382)222929
Fax: +91(02382)221149

Ref: Dscl/chem./ICCSHIP/01/2024-25 **Date: 25 / 01 /2025**

MESSAGE

Dear Esteemed Participants,

We warmly welcome you to the International Conference on Chemistry for Society, Health, Industries & Pharmacy (ICCSHIP-2025) at Dayanand Science College, Latur, India. We are thrilled to have you join us from across the globe, sharing your expertise, research, and experiences in chemistry. Your presence will enrich our discussions, foster meaningful connections, and pave the way for future collaborations.

The advantage of attending conferences is: You can connect with peers and colleagues from around the world, which can lead to future collaborations and career prospects. Conferences offer educational sessions like panels, poster sessions, and seminars, where you can learn from experts in your field. Participants can meet researchers from other countries and work on joint initiatives, grant applications, and research collaborations. Presenting at a conference can show your passion, confidence, and communication skills, which can be attractive to recruiters.

You can gain exposure to potential career paths in academia and industry. Presenting your research findings at a conference can help you hone your communication and presentation skills. You can learn to accept and understand cultural differences and thought processes. You can learn from people from a wide range of backgrounds. Let us come together to advance chemical sciences, address global challenges, and create a better future.

Thank you for your participation.

Best regards.

Yours Sincerely,

R.S Shinde

Prof. R. S. Shinde
Organizing Secretary,
(ICCSHIP-2025)

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International Conference on Chemistry for Society, Health, Industries & Pharmacy (ICCSHIP-2025)

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KEYNOTE SPEAKER

Green Synthesis of *Aegle marmelos* (Bael) Fruit Extract Nanoparticles for Sustainable Agriculture

Prof. Ganeshalingam Sashikesh,
Professor in Chemistry, Department of Chemistry, Faculty of Science,
University of Jaffna, Jaffna, Sri Lanka

Nanoparticles, renowned for their unique properties and diverse applications, necessitate careful consideration of their synthesis methods. Traditional approaches often involve hazardous chemicals and high energy consumption. Nanobiotechnology, integrated with green chemistry principles, offers a promising sustainable alternative. This approach leverages natural resources, such as plant extracts, to synthesize nanoparticles. Biologically active compounds within these extracts act as reducing, stabilizing, and capping agents, facilitating one-step nanoparticle synthesis. Green synthesis minimizes environmental impact and enhances safety compared to traditional methods. Notably, green synthesized nanoparticles, particularly silver and gold, exhibit significant potential in medicine, pharmaceuticals, and agriculture. This environmentally friendly approach reduces the use of toxic chemicals and energy, contributing to sustainable and efficient nanoparticle production. This research investigates the green synthesis of diverse nanoparticles (NPs), including silver, gold, silver oxide, and polymer NPs, utilizing *Aegle marmelos* (Bael) fruit extract as both a reducing and stabilizing agent. The synthesized nanoparticles (NPs) were characterized using X-ray crystallography (XRD), scanning electron microscopy (SEM), Fourier Transform Infrared Spectroscopy (FT-IR), and Ultraviolet-Visible (UV-Vis) absorption spectroscopy to determine their size, shape, and surface properties. UV-Vis spectroscopy confirmed the formation of AgNPs, AuNPs, and AgONPs with characteristic peaks at 421 nm, 523 nm, and 428 nm, respectively. This research focuses on evaluating the phyto-stimulatory effects, antimicrobial properties, and organic pollutant remediation potential of synthesized nanoparticles. Importantly, the study demonstrates a clear inhibitory effect of nanoparticle concentration on both microbial activity and spore production. The study also includes a brief review of nanoparticles' applications in water treatment and the development of eco-friendly nano-fertilizers, nano-pesticides, and nano-herbicides.

Keywords: Green synthesis, nanoparticles, bio-based materials, agriculture, pesticides, fertilizers, biosensors, plant growth.

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978-93-6342-558-3

New Research Trend in Chemistry and Brief Overview of Research at Central Department of Chemistry Tribhuvan University, Nepal

Prof. Dr. Megh Raj Pokhrel
Central Department of Chemistry, Tribhuvan University, Kirtipur, Kathmandu, Nepal
e-mail: meghrajpokhrel2000@ymail.com

This study will highlight the emerging research areas in chemistry, including energy, the environment, and medicine. Sustainable sources, energy-storing materials, low-cost chemically modified biomaterials for heavy metal removal, the synthesis of metal oxide nanoparticles using a green approach, and their applications for environmental remediation will be discussed briefly[1-2]. In addition, the synthesis, characterization, and photophysical studies of stimulus-responsive water-soluble polymers will be presented. Poly[n-isopropylacrylamide], Poly[NIPAM], and Poly[n-isopropylacrylamide-co-acrylic acid] (Poly[NIPAM-co-AA]) copolymers exhibit the interesting property of size contraction with increasing temperature. Photophysical probes, such as ruthenium-tris-phenanthroline and pyrene, have been used to monitor these changes, and the studies are correlated with independent steady-state fluorescence data. These novel materials are designed for use in sensor heads for the photochemical detection of pH, temperature, ionic strength, and CO_2 content in water solutions [3].

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INVITED SPEAKER

Reactions involving Sigmatropic Rearrangements-Application in the Synthesis of ICZs

Dr. Ravi Varala

Research Fellow in Health Sciences, INTI International University, Nilai campus-71800, Malaysia
& R&D Department, Scrips Pharma, Mallapur, Hyderabad-76, Telangana, India

In this talk, I discuss about the synthesis of dihydro substituted anilines involving *N*-phenyl 3-aza Cope sigmatropic rearrangements, playing with pyrazolones derivatives–controlled synthesis of six different isomers (3-aza-Cope, Claisen, base induced isomerization)and Sigmatropic rearrangements involving dioxime systems, eg. In the synthesis of Tamiflu® (Oseltamivir) and *N*-hydroxy imidazole derivatives. In addition, will discuss on how sigmatropic rearrangements will help in the synthesis of biologically relevant larger natural products, eg. indolo[2,3-á]carbazole (ICZ) glycosides.

The purpose of the talk is to enlighten research community, how photo/thermal chemistry catalyzes the reaction pathway and selectivity towards obtaining selectively one isomer/compound. This talk fits in the The United Nations (UN) designed Sustainable Development Goal (SDG) 3 [**Good health and well-being**].

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Synthesis of Kaitocephalin: A Potential Anti-Glutamate Receptor Therapeutic for Neurodegenerative Disorders

Prof. Dr. Nandkishor S. Chandan
D.Phil. (Ph.D.) Oxford University, England,
Professor and Head, Department of Chemistry,
Siddharth College of ASC, Mumbai. (University of Mumbai)

Kaitocephalin, a naturally occurring glutamate receptor antagonist, has garnered significant interest for its potential neuroprotective properties in the treatment of neurodegenerative diseases such as Parkinson's and Alzheimer's. This study focuses on the synthesis of Kaitocephalin, its structural elucidation, and its biological evaluation as a therapeutic agent. The synthetic strategy employed an efficient and scalable route, incorporating stereoselective steps to construct the complex molecular framework of Kaitocephalin. Pharmacological assays demonstrated that Kaitocephalin effectively modulates excitotoxic glutamate signaling by selectively inhibiting ionotropic glutamate receptors, a mechanism implicated in neuronal damage in both Parkinson's and Alzheimer's diseases. Preclinical studies on neuronal cell lines and animal models revealed its ability to reduce oxidative stress, inhibit neuronal apoptosis, and improve cognitive and motor function. This research highlights the potential of Kaitocephalin as a promising therapeutic agent for neurodegeneration and underscores the importance of targeting glutamate receptor pathways in the development of treatments for Parkinson's and Alzheimer's diseases. Future studies will focus on optimizing the compound's pharmacokinetics and exploring its synergy with existing treatments.

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Advanced Materials for Futuristic Applications: Innovations and Opportunities

Dr. B. N. Dole
Professor & Ex-Head
Advanced Materials Research Laboratory, Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Chh. Sambhajinagar 431004, M.S., India
Corresponding Email: drbndole.phy@gmail.com

The rapid advancements in material science have opened new frontiers for developing innovative materials tailored for cutting-edge applications in energy, environment, healthcare, and beyond. My talk will delve into the pivotal role of advanced materials, including 2D nanomaterials, graphene-based composites, and functionalized nanostructures, in shaping the future of technology. These materials exhibit remarkable properties such as superior mechanical strength, high electrical conductivity, tunable bandgaps, and exceptional chemical stability, making them ideal candidates for next-generation supercapacitors, photocatalysts, antibacterial agents, and sensors. Drawing from recent breakthroughs, including our research on graphene oxide-based nanocomposites doped with transition metals, I will highlight the synthesis, characterization, and functionalization strategies that enable these materials to achieve optimal performance in energy storage and solar energy harvesting. Special emphasis will be placed on tailoring material properties to achieve enhanced efficiency, sustainability, and scalability for practical applications. This presentation will provide insights into the growth mechanisms, structure-property relationships, and the future direction of material design and engineering. By addressing current challenges and opportunities in advanced materials, this discussion aims to inspire innovative solutions that will drive technological advancements in the years to come.

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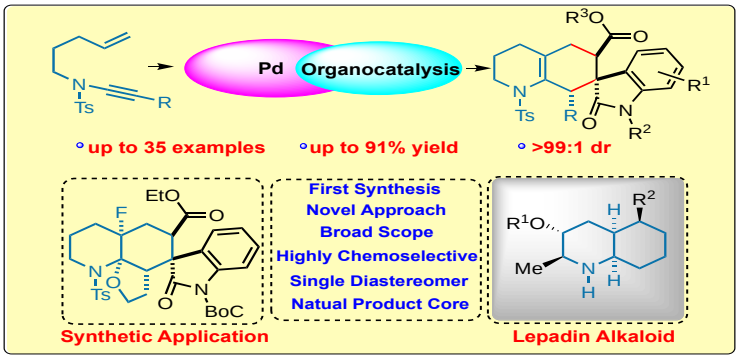
Highly Diastereoselective Synthsis of Perhydroquinoline Cores of Lepadin Alkaloids from Enynamides and Oxindoles

Dr. M. Shiva Prasad
Assistant Professor (Stage-3),
School of Basic & Applied Sciences, Central University of Tamil Nadu,
Pin. 610 005, Thiruvarur, Tamil Nadu, India. , E-mail: shivaprasad@acad.cutn.ac.in

This presentation addresses the synthesis of octahydroquinoline frameworks through a Pd-catalyzed enynaminde cycloisomerization and by an amine-catalyzed Diel's-Alder reaction sequence, in a highly stereoselective fashion. The method culminates the synthesis of >35 examples of the targeted adducts, achieving high yields and exceptional diastereoselectivity (>99:1 dr). Furthermore, the practical applicability of this approach is demonstrated *via* a two-pot, three-step procedure resulting in spiro-, tricyclic decahydroquinoline architecture that closely resemble Lepadin palkaloids.

Keywords: Cycloisomerization, Organocatalysis, Diel's-Alder, Stereoselectivity, Alkaloids.



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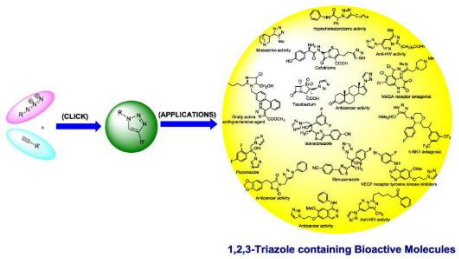
Medicinal Chemistry of 1,2,3-Triazoles: From Synthesis to Therapeutic Applications

Dr. Kishan P. Haval
Associate Professor, Department of Chemistry
Dr. Babasaheb Ambedkar Marathwada University, Chh. Sambhajinagar,
Sub Campus, Dharashiv-413501 (MS) India, Email: havalkp@gmail.com

1,2,3-Triazoles are a class of five-membered heterocyclic compounds known for their broad spectrum of biological activities. These structures can be efficiently synthesized in high yields, even on a multigram scale, through the use of click chemistry, involving the reaction of aryl/alkyl halides, alkynes, and sodium azide under mild, ambient conditions. This scaffold has received significant interest in the scientific community worldwide due to its considerable potential in drug discovery. This lecture aims to provide an overview of the current synthetic strategies for 1,2,3-triazoles and highlight their medicinal significance, particularly as lead compounds in the development of drugs.



1,2,3-Triazole containing Bioactive Molecules

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DBUH+I_3 as Novel Catalysis for Synthesis of Small Heterocyclic Molecules

Pramod Kulkarni
Professor & Head
Department of Chemistry & Post Graduate Research Center in Organic Chemistry
Hutatma Rajguru Mahavidyalaya, Rajgurunagar, Pune-410505
*Corresponding Email: pramodskulkarni3@gmail.com

We have synthesized and characterized the new amine-iodine complexes and their application as catalysts in forming diverse heterocyclic compounds. These complexes were identified through spectroscopic techniques, and physicochemical properties were studied. Among the various amine-iodine complexes screened, $DBUHI_3$ was found as the most effective catalyst for promoting the synthesis of heterocycles, including benzimidazole, benzothiazole, 2,4,5-trisubstituted imidazole, arylidene isoxazole, arylidene pyrazole, heterocyclic Schiff's base, flavone, aza-flavone, dihydropyridine, and dihydropyrazole. Reactions were optimized in various solvents, leading to a process-optimized protocol. The structures of the synthesized compounds were confirmed using spectroscopic methods such as FT-IR, ^{1}H-NMR, ^{13}C-NMR, and HRMS. Key signals in these spectra validated the fundamental skeletons of the derivatives, with some confirmations reinforced by physical constants when compared to reported molecules. Overall, this work introduces new AmineH-Iodide complexes as efficient catalysts for organic transformations, supported by optimized protocols for high-efficiency synthesis.

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Sustainable Development in Organic Reactions: Addressing Environmental and Safety Challenges

Prof. R P. Pawar
Department of Chemistry
Shiv Chhatrapati College, Chhatrapati Sambhaji Nagar, Maharashtra, India (MS) India
Email: rppawar@yahoo.com.

In recent years, the development of sustainable processes in organic chemistry has become an essential focus of research and innovation, driven by increasing concerns about environmental safety, pollution, and the use of hazardous chemicals. Traditional organic reactions often involve the use of toxic reagents, solvents, and energy-intensive procedures that contribute to environmental degradation, safety risks, and waste generation. As a result, there has been a growing need to transition towards greener, more sustainable alternatives.

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Conference Topics

- Chemistry, Education, Society,
- Organic synthesis and Methodology
- Environmental and Green Chemistry
- Natural Products & Polymer Chemistry
- Pharmaceutical and Pharmacology
- Nano science & Materials Chemistry
- Forensic and Clinical Chemistry
- Industrial Chemistry and Engineering
- Sugar and Alcohol Technology
- Coordination & Industrial Pollution
- Chemical Recycling of Waste
- Bioanalytical Chemistry
- Developments in Green Synthesis
- Photochemistry & Photo catalysis
- Bio-organic Medicinal Chemistry
- Computational and Click Chemistry
- Drug Design & Development
- Agrochemicals & Petrochemicals
- Soil and Agricultural Chemistry

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Abstract ID: ICCSHIP-2025/A-001

A Practical and Cost-Effective Approach for the Treatment of Ringworms and Ticks in Cattles

Sonkamble Mahesh Shivraj, Panchal Rutuja Kashinath
Dayanand college of Pharmacy, Latur
e-mail: maheshsonkamble447@gmail.com

Abstract: The polyherbal body wash & polyherbal body spray is beneficial for the health & the treatment of ringworms and ticks in domestic animals. The aim of the study was to formulate & evaluate, a body wash & body spray containing a natural plant extract. The formulations contain easily available plants extracts having Antibacterial, Anti-fungal, Anti-ascaracidal, and Antiinflammatory activity. The formulation of the bodywash & spray containing the above plant extracts. The physiochemical evaluation of the formulation involving PH, Viscosity, Density, Evaporation time and Spray angle, Volume actuated on each spray, Antiticks and antifungal activity. Public survey were conducted in 20 farmers to check the effectiveness of the drug on the different domestic animals specially on the cattle's & buffalo and collected their feedback and it was found that the formulation rated 9.45/10 ratings.

Keywords: Antibacterial, Anti-inflammatory, Antiticks and Antifungal

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Abstract ID: ICCSHIP-2025/A-002

Application of Preservative in Gel formation

Aakash S. Singare
School of Chemical Sciences, S.R.T.M. University, Nanded
E-mail: aakashsingare123@gmail.com

Abstract: According to Ayurvedic literature, Aloe vera is effective in treating various ailments such as fever, colic, indigestion, worm infestation, splenomegaly, and liver disorders. Additionally, it serves as a powerful detoxifier and immune booster. Aloe vera, commonly referred to as Curaçao Aloe or Barbados Aloe, is widely used in herbal medicine. The plant plays a significant role in Ayurvedic, Homeopathic, and Allopathic medicine. Aloe vera leaves are rich in numerous amino acids, natural sugars, vitamins, enzymes, and minerals. The plant exhibits purgative, antimicrobial, anti-inflammatory, antioxidant, aphrodisiac, anti-helminthic, antifungal, antiseptic, and cosmetic properties. Aloe vera juice is known for its ability to heal sunburns, burns, minor cuts, acne, and skin cancer, as well as to provide glowing, youthful skin.

Keywords: Aloe vera, citric acid, healthy and glowing skin`

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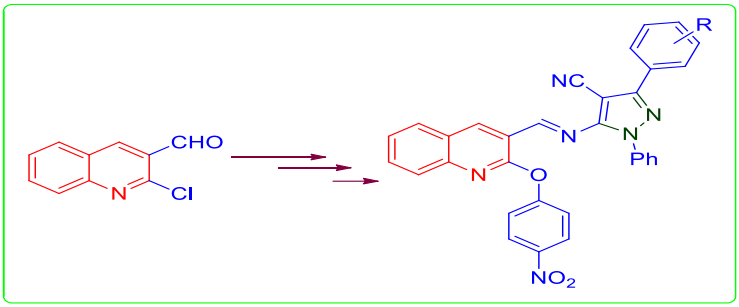
Abstract ID: ICCSHIP-2025/A-003

Synthesis and Biological Evaluation of Quinoline Linked Pyrazole Derivatives as Potent Antitubercular Agents

Somesh S. Salunke, Abhishek K. Khanzode, Kishan P. Haval*
Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Sub Campus, Dharashiv-413501 (MS) India
Email: havalkp@gmail.com

Abstract: Tuberculosis (TB) is the second leading cause of death from infectious disease and was declared a global public health emergency by the World Health Organization (WHO). Owing to the seriousness of tuberculosis various pharmacological agents have been developed. Schiff bases are a proven moiety in antitubercular drug discovery and the antitubercular drug development. Drug discovery is a never-ending process due to evolving drug resistance by the bacteria; as a result, there is a need of developing new antitubercular drugs. In continuation with our efforts towards discovery of new antitubercular agents, herewith we have reported a series of quinoline linked pyrazole derivatives. These synthesized compounds were characterized by using different spectroscopic techniques. The in vitro biological screening of target molecules against the *Mycobacterium tuberculosis* offers potent antitubercular molecules owing comparable activity to reference drugs. Our finding indicated that these newly synthesized compounds may considered as potent antitubercular drugs against the tuberculosis.



Keywords: Quinoline, Pyrazole, Schiff base**,** Antitubercular activity.

Abstract ID: ICCSHIP-2025/A-004

InCl3 Catalyzed Synthesis of O, O-Diethyl Phosphorothioates

Rajkumar U. Pokalwar
Department of Chemistry, Degloor college, Degloor, S. R.T. M. University, Nanded- 431717 (M.S.) India.
E-mail: rajupokalwar@rediffmail.com

Abstract: A simple and effective method was developed for the synthesis of O,O-diethyl phosphorothioates (3a-h) from 2-chloroquinolin-3-yl-methanol derivatives (2a-h) and O,O-diethyl phosphorochloridothioate. The reaction was performed at room temperature with indium chloride

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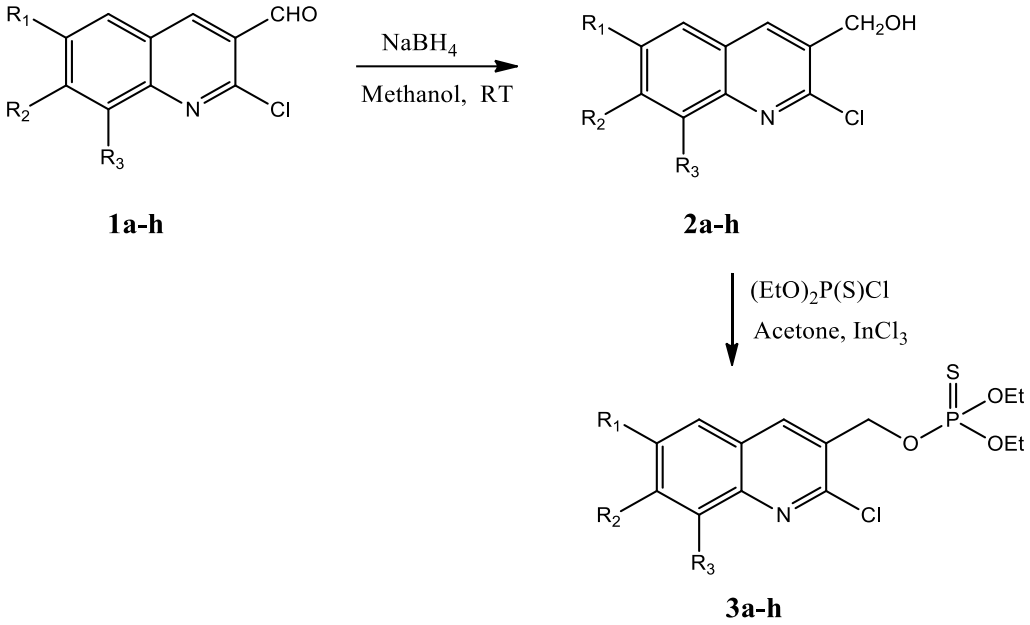
(InCl3) as a catalyst, leading to high yields of the product. The process was carried out under mild conditions with short reaction times. The resulting compounds were characterized using IR, 1H NMR, and mass spectrometry.



1a-h **2a-h**

3a-h

Abstract ID: ICCSHIP-2025/A-005

Molecular Iodine Mediated Three-Component Reaction, Synthesis of Thiadiazolo [2, 3-b] Quinozolin-6(7H)-one Derivatives in One Pot Manner

A. E. Mude[1], S.R. Sutar[1], S. M. Survase[2], A. M. chougule[1] , S. N. Ibatte[1] & J. A. Angulwar *1

[1] P. G. Department of Chemistry, Dayanand Science College, Latur (M.S.) India.

[2] P. G. Department of Chemistry, S. C. S. College, Omerga, Dharashiv (M.S.) India.

E-mail: jaangulwar@gmail.com

Abstract: Thiadiazolo [2,3-b] quinazolinone derivatives was efficiently synthesized via one-pot manner, in this paper we describe three component reaction of 4-Substituted 5-aryl-1,3,4-thiadiazolo-2-amine, dimedone and substituted aromatic aldehyde followed by catalytic amount molecular iodine in acetonitrile. The present work more convenient because reactions are taking less time and isolation of compound is easy. All reaches having excellent yields with economically chief catalyst. The synthesized compounds were characterized by IR, 1H NMR and mass spectral analysis.

Keywords: Dimedone, 1,3,4-thiadiazole, aromatic aldehyde, molecular iodine.

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Abstract ID: ICCSHIP-2025/A-006

Design, Synthesis, and Biological Evaluation of Pyrazoline Derivatives as an Anticancer Anti-inflammatory, and Antioxidant agents

Amreen N. Khalifa [a], Ganesh B. Pandhare [a], Ifat T. Dafedar [a], Sadanand N. Shringare [a] *
[a] Medicinal Chemistry Research Laboratory, School of Chemical Sciences, Punyashlok Ahilyadevi Holkar Solapur University, Solapur-413255, Maharashtra, India.
E-mail: Pandhareganesh510@gmail.com

Abstract: Three groups of novel analogs of Combretastatin-A4 (CA-4), viz., the N^1-Phenyl-pyrazoline **(5a-e),** N^1-alkyl acetylated pyrazoline **(6a-c),** and N^1-phenyl acetylated pyrazoline **(7a-g)** were designed, and synthesized in good yield. The structure of the compounds was confirmed by spectroscopic techniques. All the compounds were evaluated for their *in vitro* anticancer (MCF 7 cell line), antioxidant (DPPH, NO, SOR, and H_2O_2), and anti-inflammatory activity. Compounds **5d, 7g, 7f, 7e, 7c, 5b, 6a, 7b,** and **7a** showed excellent potency with GI_{50} ranging from **0.1 to 10.9 µM** against the MCF 7 cell line. Compounds **7f, 7g, 5c, 5d, 5b, 7e** and **6a** exhibited good anti-inflammatory activity. Encouraged by this, all the compounds were tested for their antioxidant potency. Compounds **6a, 6c, 7b, 7c, 7f, and 7g** were found to be excellent scavengers of all four free radicals (DPPH, NO, SOR, and H_2O_2).

Keywords: Anticancer, GI_{50}, Antioxidant, Pyrazoline, Anti-inflammatory

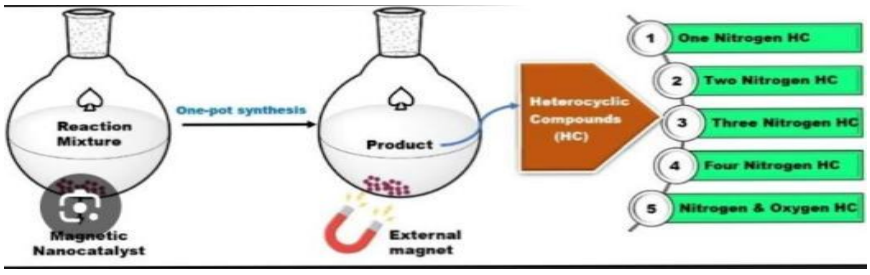
Abstract ID: ICCSHIP-2025/A-007

Chemistry of Catalyst (Synthetic and Natural)

Archana Adyappa Kumbhar [1], Mayuri Gurunath Awalkonde [1], Dhekane N.S[1]*,
[1]Department of Chemistry, Dayanand Science College, Latur 413512- Maharashtra India
E-mail: archanakumbhar060@gmail.com

Abstract: In this work, starch nanoparticles as a green and cheap catalyst were obtained based on the precipitation of amorphous starch in ethanol. It was found that starch Nanoparticles are efficient catalyst for the synthesis of 2-aminothiazoles using methylcarbonyl compounds and Thiourea as precursors. The use of green and biodegradable Nanostarch makes this present methodology quite simple, Shorter reaction times and milder conditions, and more Convenient and economically viable compared to catalyzed Methods reported in the literature

Keywords: Anticancer, GI_{50}, Antioxidant, Pyrazoline, Anti-inflammatory



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Abstract ID: ICCSHIP-2025/A-008

Synthesis of Thiouracil Derivative by Using L-Proline as a Catalyst

D. V. Hillal[1], M. P. Munde*[1]
[1]Department of Chemistry, Dayanand Science College, Latur 413512- Maharashtra India
E-mail: mmunde418@gmail.com

Abstract: This project explores the synthesis of thiouracil derivatives using L-proline as an eco-friendly organocatalyst. Aromatic aldehydes, ethyl cyanoacetate, and thiourea were reacted in ethanol under reflux, monitored via TLC. The derivatives were isolated by precipitation and characterized by melting points. The results showed L-proline achieved up to 90% yields under mild conditions, with advantages such as simplicity, availability, and environmental safety. These derivatives hold potential for biological applications, demonstrating a sustainable method for advancing pharmaceutical research.
Keywords: L-proline, thiouracil derivatives, thiourea, aldehydes

Abstract ID: ICCSHIP-2025/A-009

The Role of Regulatory Affairs in Pharmaceutical Drug Development

Waghmare R. S, [1] Shinde P. D, [1] Khandomalke V. R.[1]
[1]Dayanand College of Pharmacy, Barshi Road, Latur, 413512, Maharashtra India
E-mail: vaishnavikhandomalke@gmail.com

Abstract: The pharmaceutical industry is highly regulated to ensure the safety, efficacy, and quality of therapeutic products. Regulatory Affairs (RA) serves as the backbone of this system, managing the interface between regulatory authorities, drug developers, and other stakeholders. This paper explores the essential contributions of RA throughout the drug development lifecycle, from preclinical research and clinical trials to regulatory submissions and post-marketing surveillance. By ensuring compliance with global regulatory standards, RA plays a vital role in expediting drug approvals while maintaining public health.
Keywords: RA, preclinical research, clinical trials, post-marketing surveillance

Abstract ID: ICCSHIP-2025/A-010

Formulation and Evaluation of Memory Booster Chocolate for Pediatrics

Divya Bawaskar
School of Pharmacy, Swami Ramanand Teerth Marathwada University, Nanded-431606
*Email: divyabawaskar11@gmail.com

Abstract: The chocolate is most loving food of children whereas medicine is hating substance. So, the objective of this study is to fabricate and design chocolate. The essential target of this study was to formulate and evaluate memory booster chocolate and nutritional supplement containing antioxidant and other property. Chocolate is a range of products derived from cocoa (cocoa) mixed with fat and finely powered coconut sugar to produce a solid confectioner. The chocolate provides

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smooth and creamy texture to the formulation and are good for masking the unpleasant taste associated with some drugs.

Keywords – Trichomonas vaginalis, Neisseria gonorrhoeae, HRLCMS analysis, Molecular docking

Abstract ID: ICCSHIP-2025/A-011

Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery-A Review

Mrs. Shazia Farheen[1], Mr. Sumit Joshi[1]
[1]Department of Computer Science, Dayanand Science College, Latur
Maharashtra, India
*Email: shazia41@gmail.com, mr.joshi.sumit@gmail.com

Abstract: The term "artificial intelligence" was introduced by John McCarthy in 1956 at Dartmouth Conference, defining it as "the science and engineering of making intelligent machines." This foundational definition remains relevant, though further details have been added over time. AI, a field drawing from numerous disciplines, incorporates knowledge from areas like computer science, mathematics, psychology, linguistics, philosophy, neuroscience, and more. Although AI has existed for some time, its application to drug discovery, particularly in modeling structure-activity relationships, is not recent. Hansch is often called the "father of QSAR" within pharmaceuticals. Since then, an increasing number of medicinal chemists have used AI techniques to assess and predict how chemicals impact biological systems. AI is increasingly being used in nearly all stages of early drug discovery, from identifying targets and finding potential drug candidates to optimizing leads, predicting properties and toxicity, and even structuring clinical trials.

In this paper, we perform a review study of Developing innovative small-molecule drugs is a challenging process, plagued by high costs, low clinical trial success rates, and lengthy development timelines. A key obstacle in medicinal chemistry is bridging the gap between basic scientific discoveries and early clinical trials. While researchers now have unprecedented access to vast amounts of data, integrating this information effectively into their work remains a hurdle. One potential solution lies in leveraging machine intelligence to analyse complex, multifaceted data. Therefore, machine learning and domain-specific AI present promising avenues for advancing small-molecule drug discovery. Significant advancements have been made in machine learning algorithms and their applications. This review will highlight the proven applications of AI in this area and explore the most promising technologies for the next generation of AI-driven drug discovery.

Key words: Artificial Intelligence, Machine learning, AI-driven drug Discovery, Applications of AI

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Abstract ID: ICCSHIP-2025/A-012

Isolation, Characterization and Identification of Bacillus Megaterium Ra-Fi7

Dr. F. S. Biradar[1], Dr. V. S. Shembekar[2]
[1]Department of Biotechnology, Dayanand Science College, Latur.
[2] Department of Zoology, Rajarshi Shahu College, Latur.
E-mail: firdousbiradar@gmail.com

Abstract: The present study aimed to isolate, characterize, and identify a potential Phosphate solubilising bacteria Bacillus megaterium, a prominent Gram-positive bacterium with significant industrial, agricultural, and environmental applications. Soil samples were collected from various agricultural fields with the objective of isolating bacterial strains capable of contributing to biofertilization and bioremediation processes. The isolation process involved the use of selective media that supported the growth of B. megaterium, ensuring the successful separation of this microorganism from the native microbial population. Initial characterization included morphological observation, where colonies exhibited large, creamy-white, circular appearances typical of B. megaterium. Microscopic examination confirmed the presence of large, rod-shaped cells, and Gram-staining verified their Gram-positive nature. Further biochemical tests, including catalase production, starch hydrolysis, and nitrate reduction, aligned with the expected profile of B. megaterium. The bacterium's ability to produce extracellular enzymes like protease and amylase was evaluated, indicating its potential in industrial enzyme production. For molecular identification, 16S rRNA gene sequencing was employed, confirming the isolate as Bacillus megaterium. Phylogenetic analysis also supported the identification by placing the isolate within the Bacillus genus. The versatility of B. megaterium in producing bioactive compounds, along with its ability to survive in extreme conditions, highlights its potential for applications in agriculture as a biofertilizer and in environmental sectors as a bioremediating agent. This study not only advances the understanding of Bacillus megaterium in biotechnological and ecological settings but also opens new avenues for further exploration of its beneficial roles in sustainable agricultural practices and environmental management.

Keywords – Bacillus megaterium, isolation, characterization, identification, 16S rRNA sequencing, biofertilizer, bioremediation, enzyme production, soil bacterium, Agricultural Microbiology.

Abstract ID: ICCSHIP-2025/A-013

Enstioselective Synthesis of 4-Nitroalkyl-1H-Indol-5-ol Through Asymmetric Catalytic Reaction Using DPPTT as Organocatalyst

Hanmant M. Kasralikar
Department of Chemistry, Lal Bahadur ShastriMahavidyalaya, Dharmabad-431809, MS, India
*Email: hanmantkasralikar@gmail.com

Abstract: The heteroaryl substituted derivatives incorporating an indole core has applications in medicinal, agrochemical and material sciences due to this it represents an important class of heterocyclic compounds. The enantioselective synthesis of this kind of compounds constitutes a

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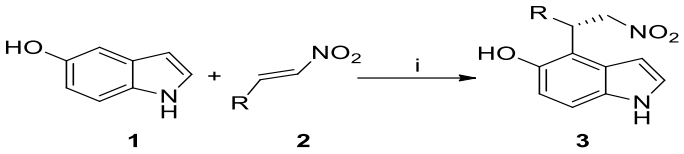
major theme of recent research using asymmetric catalytic reactions (ACR). Nitroalkanes of heterocyclic compound has valuable importance as an intermediate in organic synthesis; we intended a method for the synthesis of asymmetric 4-nitroalkyl-indol. The procedure involves the introduction of an indole framework in the β-position of a nitro styrene via a Friedel–Crafts alkylation



Reaction conditions: i) DPPTT(5mol%), EtOH(10ml), Stir, at 60oC, 85-90% yield, 80-95% ee

Abstract ID: ICCSHIP-2025/A-014

Synthesis of Various 1, 5-Benzodiazepines Derivatives and Studied Their Antimicrobial Activity

Kendre Madhav Marotirao
Department of Chemistry, Shri Sant Gadge Maharaj Mahavidyalaya, loha Tq. Loha Dist. Nanded-431708 Maharashtra, INDIA
*Email: madhavkendre72@gmail.com

Abstract: In recent time millions of heterocyclic compounds were synthesized due to their specific activity are employed in the treatment of many infectious diseases. Their use in the treatment is attributed to their inherent toxicity of various pathogens. Among a wide range of heterocyclic compounds that have been explored for the development of pharmaceutically important molecules. Most of the heterocyclic compounds are well known due to their biological importance. Out of these 1, 5-benzodiazepines are important seven member heterocyclic molecules which represent a variety of biological activities. A series of-2, 4-(substituted-phenyl)-2, 3-dihydro-1H-1, 5-benzodiazepine derivatives (2a-j) have been synthesized by the treatment of 1-(substituted-2-hydroxy-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (1a-j) with 4-methyl-ortho-phenylene diamine and few drops of piperidine using 20 ml methanol as a solvent was refluxed for 4 hrs. Then glacial acetic acid (5 ml) was added to the reaction mixture and refluxing was continued for 2 hrs, after completion of reaction (checked by TLC). The reaction mixture was left overnight at room temperature. In 70-80% yield with high purity, characterization of compounds was confirmed by the IR, 1H NMR and mass spectral analysis. All these newly synthesized compounds were evaluated for their antibacterial activity against four different pathogens such as Escherichia coli, Salmonella typhi, Staphylococcus aureus and Bacillus subtilis and antifungal activity against Aspergillus niger, Penicillium chrysogenum, Fusarium moneliforme and Aspergillus flavus, using Penicillin and Greseofulvin using Peniciline and Greseofulvin as standard drugs by agar cup method and Poison plate method, respectively.

Keywords: 2-Hydroxy-chalcones, ortho-phenylene diamine, 1, 5-Benzodiazepines, Antimicrobial activity.

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Abstract ID: ICCSHIP-2025/A-015

Development and Validation of an Rp-Hplc Method for the Estimation of Anticoagulant Drug in Tablet Dosage Form.

Mahesh Mali*, Revan Karodi , Kunal Warwatkar
Dr. D Y Patil College of Pharmacy, Akurdi.
*Email: madhavkendre72@gmail.com

Abstract: The development and validation of a robust, precise, and accurate Reverse-Phase High-Performance Liquid Chromatography (RP-HPLC) method for the estimation of anticoagulant drugs in tablet dosage forms is critical to ensuring quality control and compliance with pharmaceutical standards. This study aims to establish a simple, sensitive, and reproducible RP-HPLC method for the quantitative analysis of a selected anticoagulant drug. The method was optimised and validated in accordance with International Council for Harmonisation (ICH) guidelines, focusing on parameters such as linearity, precision, accuracy, robustness, and specificity.

The chromatographic separation was achieved using a C18 column (250 × 4.6 mm, 5 µm particle size) with a mobile phase comprising a mixture of phosphate buffer (pH 4.5) and acetonitrile in a ratio of 60:40 v/v, at a flow rate of 1.0 mL/min. The detection wavelength was set at 260 nm, and the retention time of the drug was found to be approximately 6 minutes. The method exhibited excellent linearity in the concentration range of 5-50 µg/mL, with a correlation coefficient (R^2) greater than 0.999. The precision, expressed as %RSD, was less than 2%, indicating high reproducibility. Accuracy studies demonstrated recovery rates between 98.5% and 101.5%, confirming the method's reliability. The method was also found to be robust under slight variations in chromatographic conditions.

The validated RP-HPLC method was successfully applied to the estimation of the anticoagulant drug in commercial tablet formulations, with results consistent with labeled claims. This method provides a reliable tool for routine quality control analysis of anticoagulant drugs in pharmaceutical industries.

Keywords:- RP-HPLC, Edoxaban, Anticoagulant, Method Development, Validation, ICH Guidelines, Chromatographic Separation, Pharmaceutical Analysis, Quality Control, Precision, Sensitivity, Robustness.

Abstract ID: ICCSHIP-2025/A-016

Sustainable Agriculture Through Biopesticidal Applications of Annona Squamosa Seed Extracts

Mitali Sonkamble[1]
[1]Dayanand College of Pharmacy, Latur. -413512, Maharashtra, India
E-mail: mitalisonkamble@gmail.com

Abstract: The increasing environmental and health concerns associated with synthetic pesticides have driven interest in natural, eco-friendly alternatives. Custard apple (Annona squamosa) seeds are a promising source of biopesticidal compounds due to their rich phytochemical profile,

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including acetogenins and alkaloids, known for their insecticidal properties. This study evaluates the biopesticidal efficacy of custard apple seed extracts against common agricultural pests.
Seed extracts were prepared using various solvents (e.g., ethanol, methanol, and water) and tested for their pest control activity under laboratory conditions. Results demonstrated significant mortality rates in target pest species, with ethanol extracts exhibiting the highest efficacy. Phytochemical analysis revealed the presence of bioactive compounds responsible for the observed activity.
The findings suggest that custard apple seed extracts hold great potential as an eco-friendly and sustainable alternative to synthetic pesticides, offering benefits for integrated pest management strategies. Further research is recommended to assess field-level efficacy and environmental safety.

Abstract ID: ICCSHIP-2025/A-017

Novel Diagnostic Kit for the Detection of Vaginal Candidiasis: Sanitary Pads.

Prakash Honrao, Sonali Korale, Mohini Patil
Dayanand College of Pharmacy, Latur
*Email: prakashhonrao1122@gmail.com

Abstract: There are at least two challenges for women living in poor countries, having symptoms of vaginal candidiasis. First, they may lack access to healthcare facilities where a vaginal swab could be taken and antifungal medicine could be dispensed. Secondly, societal taboos may prevent them from telling other people about their symptoms. Keeping these limitations in mind, we try to develop diagnostic sanitary napkins that would allow females to self-diagnose such infections. In this research newly designed menstrual hygiene products enable easier and economical detection of vaginal candidiasis. The sanitary napkin produces coloured spots while coming in contact with the vaginal secretions of infected females. Detection can be done quickly within ten minutes, and the cost is much lesser in comparison with standard tests. With this the present study also prevents the misdiagnosis and unnecessary use of OTC antifungal drugs.
Keywords: Sanitary napkins, cotton thread, candidiasis, Diagnostic kit etc.

Abstract ID: ICCSHIP-2025/A-018

Zinc Oxide Nanoparticles Doped with Graphene for Dye Sensitized Solar Cells

Nidhi Gupta
Department of chemistry, Punjabi University, Patiala, Punjab-147001
E-mail: drnaveenabs@gmail.com

Abstract: Zinc oxide (ZnO) nanoparticles were synthesized via a sol-gel method and doped with graphene to enhance their photocatalytic efficiency. The integration of graphene with ZnO nanoparticles significantly improves charge separation and electron transport due to graphene's high electrical conductivity and large surface area. The composite material was characterized using XRD, SEM, and UV-Vis spectroscopy to confirm its structural integrity and optical properties. When tested for the degradation of organic pollutants under simulated solar irradiation, the ZnO-graphene composite demonstrated superior photocatalytic activity compared to pure ZnO. This

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enhancement is attributed to the synergistic interaction between ZnO and graphene, which reduces electron-hole recombination and increases the availability of active sites. The results highlight the potential of ZnO-graphene composites as efficient, sustainable photocatalysts for environmental remediation and energy applications.

Keywords: ZnO Nanoparticles, Graphene, Photocatalyst, Photo degradation, Charge Separation, Environmental Remediation

Abstract ID: ICCSHIP-2025/A-019

Phytochemical Screening and Anthelmintic Activty of Carrisa Carandas

Sainath Dalvi[1], Pankaj Chavan[1]
[1]School of Pharmacy, Swami Ramanand teerth Marathwada University, Nanded-431606, Maharashtra, India
E-mail: prakashhonrao1122@gmail.com

Abstract: The anthelmintic activity of them Ethanolic and Methanolic extract of the Leaves of Carissa carandas was evaluated on adult Indian earthworm (Pheretima posthuma) using albendazole as a reference standard. The extract caused paralysis followed by the death of worm at the tested doselevel.The phytochemical screening of the crude extract showed presence so alkaloid, tannins, flavonoids, saponins, proteins, amino acids, terpenoid, glycoside and phenolic compound.

Abstract ID: ICCSHIP-2025/A-020

Vipera Nikolskii Venom Boon Against SARS-Cov

Tikambare Saraswati Vijayanand[1]
[1]Dayanand College of Pharmacy, Latur – 413512, Maharashtra, India
E-mail: saraswatitikambare@gmail.com

Abstract: Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), the causative agent responsible for the coronavirus disease-2019(Covid-19). SARS-CoV-19 was identified in December 2019 in the Chinese city, Wuhan. Coronavirus disease is a pulmonary disease, In which local direct vascular and endothelial injury occur in the lungs and other organs leads to clot formation and angiopathy,leads to thrombosis in the pulmonary arteries (Pulmonary embolism) and arteries of brain(stroke). In severe Covid-19 patient's pulmonary embolism and stroke has been reported in 20-30% and 3-5% respectively. Peptides or antithrombotic proteins may help in covid-19. It binds to enzymes angiotensin converting enzyme 2 act as receptor, improvement in vascular function occur, it make the blood vessels relax. Vipera nikolskii venom boon against covid-19.

Keywords: SARS-CoV-2, Pulmonary embolism, Stroke, Angiotensin converting enzyme-2, Vipera nikolskii venom

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Abstract ID: ICCSHIP-2025/A-021

A Comparative Study of Ultrasonic Assisted and Conventional Synthesis of B-Diketone and It's Transition Metal Complexes

Seema Mehatre[1], Nanda S. Korde[2]*
[1]Shri Chhatrapati Shahu Maharal Sainiki Junior College, Udgir
[2]Dayanand Science College, Latur, Maharashtra, India
E-mail: nandineekorde0@gmail.com

Abstract: In ultrasonication technique ultrasonic (> 20 KHz) waves are irradiated into a liquid sample resulting in oscillation. This method is now-a-days a well-considered technology in green chemistry being advantageous over the conventional thermal methods as increased reaction rates, formation of purer products, improved yield, increased selectivities, easier experimental procedures and use of milder conditions both in case of heterogenous and homogenous reactions. Here, we were synthesized β-diketone and its transition metal complexes by conventional and ultrasonic irradiation methods. Synthesized β-diketone acts as chelating agent in the preparation of transition metal complex.
Keywords: Ultrasonication, β-diketone, Metal Complexes, Time, Yield, Purity etc.

Abstract ID: ICCSHIP-2025/A-022

Influence of Salt Tolerant Trichoderma Sp. on Growth of Wheat (Triticum Aestivum) and Chickpea (Cicer Arietinum) Plant.

Dhutekar Shailaja[1], Vedpathak Deepak[2]
[1]Research Scholar, Department of Microbiology, Rajarshi Shahu Mahavidyalaya (Autonomous)
[2] Department of Microbiology, Rajarshi Shahu Mahavidyalaya (Autonomous) Latur.
E-mail: anujaav2007@rediffmail.com

Abstract: Indole-3-acetic acid (IAA), a vital phytohormone, plays a critical role in plant growth and development by regulating cell elongation, division, and differentiation. Salinity is one of the major agricultural concern that significantly limits the crop productivity. The production of IAA by salt-tolerant Trichoderma species has emerged as a promising approach for enhancing plant growth, especially in saline-affected soils. This study focuses on isolating and characterizing salt-tolerant Trichoderma strains capable of producing IAA under saline conditions. These strains were evaluated for their IAA production using biochemical and TLC technique.
Results demonstrated that the selected five Trichoderma isolates T1,T2,ST1,ST2& SC8 were identified as Trichoderma viridae,Trichoderma herzianum,Trichoderma atroviridae,Trichoderma longibrachiatum,Trichoderma Koningii respectively on the basis of 18S rRNA sequencing, produced significant levels of IAA even at 3% and 4% salt concentrations, indicating their adaptability and potential for biotechnological applications in saline environments. Furthermore, pot trials showed that applying IAA-producing Trichoderma enhanced seed germination, root elongation, and overall plant biomass in Triticum aestivum and Cicer arietinum crops. This improvement was attributed to the dual effect of IAA production and the biocontrol properties of Trichoderma, which reduced plant stress and improved nutrient uptake.

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The findings underscore the potential of salt-tolerant Trichoderma strains as bioinoculants for sustainable agriculture, particularly in saline and marginal lands. Integrating these beneficial fungi into crop management strategies can mitigate the adverse effects of salinity while promoting plant growth and productivity.

Keywords: Indole-3-acetic acid, IAA, salt-tolerant Trichoderma.

Abstract ID: ICCSHIP-2025/A-023

Formulation and Evaluation of Silver Nanoparticle Gel of Azadirachta Indica for Treatment of Acne Vulgaris

Sneha C. Kakade, Vijayendra Swamy S. M.
Principal, Channabasweshwar Pharmacy College (Degree), Latur- 413512, Maharashtra, INDIA.
E-mail: kakadesneha7@gmail.com

Abstract: Acne vulgaris is one of the most prevalent skin conditions, affecting nearly 80% of adolescents worldwide. It results from the accumulation of sebum and dead cells, which clog hair follicles, creating an environment for bacterial proliferation and inflammation. Conventional antibiotic treatments often lead to antibiotic resistance and hypersensitivity reactions. This study aimed to evaluate the phytochemical composition of Azadirachta indica, synthesize silver nanoparticles (AgNPs) using its extract, and develop a topical herbal gel formulation for acne treatment. Azadirachta indica was selected for its known antibacterial properties. Phytochemical analysis confirmed the presence of alkaloids, flavonoids, tannins, and terpenoids in the extract. AgNPs were synthesized using a 1 mM aqueous silver nitrate solution and confirmed via UV spectroscopy. The nanoparticles were stable, spherical, with an average size of 207.6 nm and a polydispersity index of 0.248. The synthesized AgNPs were incorporated into a gel base and evaluated for physical properties such as pH, viscosity, spread ability and antibacterial activity against Propionibacterium acnes and Staphylococcus aureus. The formulation exhibited uniform colour dispersion, no lumps, good washability, and spread ability. The pH values of 6.72 and 6.80 were compatible with skin pH. Antibacterial studies showed significant inhibitory activity against P. acnes and S. aureus, with AgNPs demonstrating greater efficacy than the crude extract. These findings suggest that AgNPs synthesized from Azadirachta indica incorporated into an aqueous gel base present a promising herbal formulation for acne vulgaris treatment.

Keywords: Acne vulgaris, Azadirachta indica, Silver Nanoparticles, Topical herbal gel, phytochemical analysis, Antibacterial activity.

Abstract ID: ICCSHIP-2025/A-024

Synthesis of PO_4^{2-}/ZrO_2 Solid Acid Catalyst for Organic Transformation

A. L. Ghodke[1], Dr. R. P. Barkul, Dr. S. T. Dhumal, Dr. V. S. Suryawanshi[2]*, Dr. M. K. Patil*
[1] Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Sub-campus Dharashiv- 413 501, MS, India
[2]Chhatrapati Shivaji College Omerga-413606, MS, India
E-mail: meghshyam_patil@yahoo.com

Abstract: In this investigation, PO4 2-/ZrO2 solid acid catalyst was synthesized using a simple precipitation method involving use of zirconyl nitrate and orthophosphoric acid. The resulting solid acid catalyst was characterized by various techniques, including XRD, IR, UV-Vis, TGA, SEM, and

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TEM, confirming the successful preparation of PO4 2-/ZrO2. The activity of this solid acid catalyst was demonstrated in the synthesis of a novel series of hydrazino thiazole derivatives. This synthetic strategy offers advantages such as reduced reaction times and high yields. The structures of the compounds were confirmed through IR, 1H NMR, and 13C NMR spectroscopy.

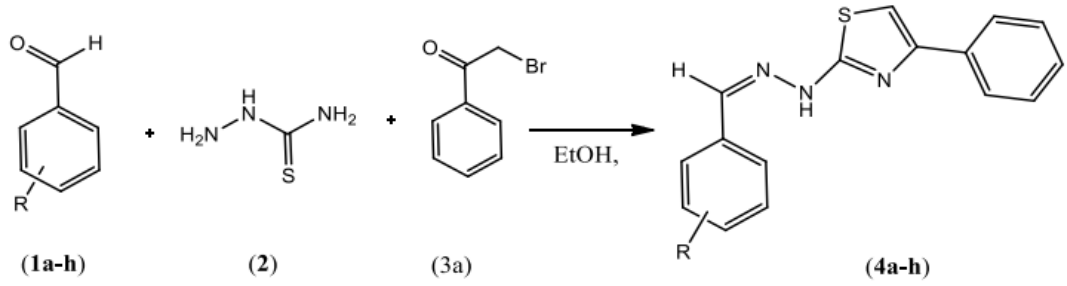

Figure 1: Synthesis of hydrazino thiazole derivative.

Abstract ID: ICCSHIP-2025/A-025

Phytochemical Screening, In Silico Studies and Several Novel Pharmacological Activities of Plant Extracts of Monoon longifolium

Rutuja Magar[1]*, Seema Gaikawad[1]*, Mrudul Dange[1], Dr. S. R.Butle[1]
[1]School of Pharmacy, Swami Ramanand Teerth Marathwada University, Nanded-431606
E-mail: rutujamagar2050@gmail.com

Abstract: Exploring the Antiparasitic Potential of Monoon longifolium Leaf Extracts against Trichomonas vaginalis and Neisseria gonorrhoeae. Trichomoniasis (Trichomonas vaginalis) and gonorrhea (Neisseria gonorrhoeae) are major sexually transmitted infections with increasing drug resistance to standard treatments like Metronidazole and Ceftriaxone, necessitating alternative therapies. This study investigates the antiparasitic properties of Monoon longifolium leaf extracts prepared using six solvents (methanol, water, glacial acetic acid, ethyl acetate, toluene, and hexane). Phytochemical analysis revealed bioactive compounds such as flavonoids, polyphenols, and alkaloids. Soxhlet extraction yielded the highest extractive efficiency with ethyl acetate (7.92%) and glacial acetic acid (10.6%). High-resolution LC-MS identified 63 compounds in the ethyl acetate extract, including 3-O-trans-Feruloyleuscaphic Acid and Ganosporelactone A. Molecular docking showed strong binding affinities of 3-O-trans-Feruloyleuscaphic Acid (-14.7) against T. vaginalis and Goyaglycoside A (-15.1) against N. gonorrhoeae. In vitro, ethyl acetate extracts exhibited significant inhibition (35 mm zone) for both pathogens, outperforming standard antibiotics. These results highlight Monoon longifolium extracts, particularly ethyl acetate and glacial acetic acid, as promising candidates for alternative treatments, warranting further research.

Keywords: Trichomonas vaginalis, Neisseria gonorrhoeae, HRLCMS analysis, Molecular docking.

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Abstract ID: ICCSHIP-2025/A-026

Chemistry of catalyst (Synthetic & Natural)

Gaikwad Anjali Sudhakar, Prof. R. K. Jadhav
Research Centre in Chemistry, Department of Chemistry, Dayanand Science College, Latur – 413512, Maharashtra, India
*Email: anjaligaikwad3922@gmail.com

Abstract: The synthesis of 2, 2'-(4-nitrophenylmethylene) bis (5, 5-dimethyl-1, 3-cyclohexanedione) involves the condensation reaction between 4-nitrobenzaldehyde and two equivalents of 5,5-dimethyl-1,3-cyclohexanedione (dimedone) under basic or acidic catalytic conditions. This reaction yields a bis-compound characterized by the methylene bridge connecting the two cyclohexanedione moieties. The product is often isolated in good yields and exhibits interesting properties, such as potential applications in dye synthesis, medicinal chemistry, or as intermediates in organic synthesis. Structural characterization is typically confirmed by spectroscopic techniques like NMR, IR, and mass spectrometry, ensuring the formation of the desired bis-dimedone derivative. This synthesis offers a straightforward approach to constructing complex organic molecules with potential biological and industrial significance. The reaction is typically catalyzed by a base such as piperidine or sodium hydroxide in an ethanol medium. The product is obtained as a crystalline solid in high yield, characterized by the formation of a methylene bridge linking two dimedone units to the nitrophenyl group. Structural confirmation is achieved through spectral analysis including FT-IR, ^{1}H-NMR, and mass spectrometry. This compound demonstrates potential utility in organic synthesis, pharmaceutical development, and as a precursor for bioactive molecules.

Keywords: Molecular Compound knoevenagel condensation, cyclohexadione derivation, nitrophenyl group organic synthesis, diketone, condensed aromatic system, UV-vis spectroscopy, chromophore, pharmaceutical Intermediate, biological activity Synthetic chemistry.

Abstract ID: ICCSHIP-2025/A-027

Formulation and Evaluation of Nanogel for the Treatment of Antifungal Disease

Nivrutti Kotsulwar, Mayur Upade
Channabasweshwar Pharmacy College (Degree) Kava Road, Basweshwar Chowk, Latur-413512
*Email: nivruttikotsulwar2050@gmail.com

Abstract: Nanogels represent a cutting-edge nanotechnology-based platform for the delivery of antifungal agents, offering significant advantages such as enhanced drug solubility, controlled release, and targeted delivery. This study investigates the formulation and evaluation of a nanogel developed specifically for the treatment of antifungal diseases. The nanogel was synthesized using a biocompatible polymer matrix, optimized for critical parameters including encapsulation efficiency, particle size, and drug loading. Antifungal agents such as fluconazole and itraconazole were effectively incorporated into the nanogel, ensuring stability and sustained drug release.
The nanogel was characterized using advanced analytical techniques, including dynamic light scattering (DLS) for particle size distribution, scanning electron microscopy (SEM) for

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morphological analysis, and Fourier-transform infrared spectroscopy (FTIR) to evaluate chemical compatibility. In vitro drug release studies demonstrated a controlled release profile, enhancing therapeutic efficacy and reducing side effects. Antifungal activity was assessed through microbiological assays against clinically significant strains, including Candida albicans and Aspergillus Niger, revealing substantial inhibition zones compared to conventional formulations.

Furthermore, cytotoxicity assessments conducted on human keratinocyte cell lines confirmed the nanogel's favourable safety profile. These findings highlight the potential of this nanogel system to transform antifungal therapy by improving drug bioavailability, reducing systemic toxicity, and enhancing patient compliance. Future investigations will focus on clinical translation and scalability of the formulation to facilitate its widespread adoption in medical practice.

Keywords: Nanogel, Antifungal Diseases, Targeted Drug Delivery, Sustained Release, Topical Therapeutics, Fungal infections, Controlled drug release, Topical therapeutic system, Enhanced penetration, Nanotechnology, Localized therapeutic action.

Abstract ID: ICCSHIP-2025/A-028

Tamarind Juice Catalyzed Cost Effective and Green Synthesis of 1, 4-Dihydropyrimidine Derivatives

Amit S. Waghmare[1]*, Kailash R. Kadam[2], Ajay N. Ambhore[3]

[1] Department of Chemistry, Arts, Commerce and Science College, Satral, Ahilyanagar, MS, INDIA

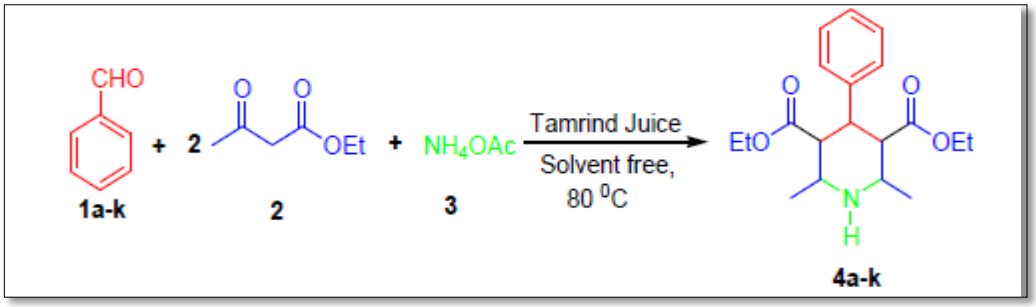
[2] Padmashri Vikhe Patil Arts, Commerce and Science College, Pravaranagar, Loni Kd., Ahilyanagar, MS, INDIA

[3] Department of Chemistry, Vivekanand College, Kolhapur (Empowered Autonomous), MS, INDIA

E-mail : asw6807@email.com

Abstract: Tamarind juice act as a cost effective and green catalyst for the efficient synthesis of 1, 4-dihydropyrimidine derivatives. This Hantzsch reaction is achieved using ethyl acetoacetate, ammonium acetate and different aromatic aldehyde at 80°C under solvent free condition. The important features of present protocol are easily available, nontoxic catalyst, solvent free condition, shorter reaction time and good to excellent yields. Operational simplicity, simple workup procedure, formation of no by-product is some of the additional features of this protocol.

Keywords: Tamarind juice, natural catalyst, solvent free condition, 1, 4-dihydropyrimidine, green synthesis.



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Abstract ID: ICCSHIP-2025/A-029

Evaluation of Skeletal Muscle Relaxant Activity of Muca Acuminata Pulp Extract In Wistar Rats

Jadhvar Ankita Sanjivan
Dayanand College of Pharmacy Latur
*Email: ankita7092000@gmail.com

Abstract: Skeletal muscle relaxant activity of the methanolic fruit pulp extract of Musa Acuminata was investigated by testing the effect of the extract on wistar rat. The evaluation of in vivo skeletal muscle relaxant activity in rats was done using rotarod model and acophotometer model Experiments were carried on female Wistar rats and the animals were randomly allotted to the different control and test groups.the powdered plant material was extracted by Soxhlet extractor in methanol and acetone. Phytochemical testing of extracts discovered presence of glycosides, flavonoids, carbohydrates tannins phenolics etc. Antioxidant activity was carried out by 2.2 diphenyl-1-picrylhyrazyl (DPPH) assay. DPPH scavenging assay were performed to evaluate the antioxidant activity which was found maximum at 50 microgram concentration for methanolic extracts. The extract was administered orally at a dose of 250 mg/kg and 500mg/kg. Diazepam in adose of 10mg/kg was used as a standard. The result showed that methanolic extract of Musa Acuminata shows significant skeletal muscle relaxant activity as compared to standard drug at the doses of 250mg/kg and 500mg/kg

Abstract ID: ICCSHIP-2025/A-030

Development and Validation of Rp-Hplc Method for Simultaneous Estimation of Gliclazide and Metformin Hydrochloride from the Tablet Dosage Form

Badagu Rajshree Shriniwas, Bhavle Urmila Shivaji
Dayanand College of Pharmacy, Latur – 413512, Maharashtra, India
*Email: badagurasjhree@gmail.com

Abstract: An efficient and simple HPLC method has been developed and validated for the simultaneous determination of Gliclazide and Metformin Hydrochloride from marketed tablet dosage form. The mobile phase used for the chromatographic runs consisted of 0.05M Phosphate buffer (pH5), Methanol and Acetonitrile (47.5:47.5:5). The separation was achieved on Agilent 5 TC – C 18 (2)250×4.6mm column. Drug peaks were well separated and were detected by a UV detector at 232 nm. The method has been validated according to the ICH guidelines Q2R1 with respect to system suitability, assay, specificity, linearity and range, precision, accuracy, and robustness. The flow rate was 1.0ml/min. The retention time of Metformin Hydrochloride and Gliclazide was found to be 2.79min and 4.26min respectively. All the validation parameters were found within the acceptable range

Keywords: RP-HPLC method validation, Gliclazide and Metformin Hydrochloride

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Abstract ID: ICCSHIP-2025/A-031

Development and Validation of Rp-Hplc Method for Estimation of Dapagliflozin in Solid Dosage Form

Surwase Mohini shivaji, Dound Aishwarya Narsing
Dayanand College of Pharmacy, Latur – 413512, Maharashtra, India
*Email: aishwaryadound@075gmail.com

Abstract: Dapaglificzin Dapagliflozin is Active pharmaceutical al ingredient ingredient mostly used in the treatment of TYPE- -2 Diabetes Mellitus. An efficient and simple HPLC method has been developed and validated for the determination of Dapagliflozin in solid dosage form. The Mobile phase used for the chromatographic runs consisted of Sodium Acetate Buffer PH 4.5 THF Methanol (30:10:60). The Separation was achieved on Agilent STC-C18 Drug peaks were separated and detected by a UV detector at 223nm. The method has been validated according to ICH (Q2 R1) quidelines with respect to system suitability, specificity, precision, accuracy and range, robustness. The flow rate was 8 min. All the validation parameters were were found within the acceptable range.
Keywords: Dapagliflozin. RP-HPLC method validation.

Abstract ID: ICCSHIP-2025/A-032

Development of a Novel Luliconazole Transferosomal Gel for Enhanced Antifungal Delivery

Kolpe Punam Sudhakar
Dayanand College of Pharmacy, Latur – 413512, Maharashtra, India
*Email: poonamkolpe18@gmail.com

Abstract: Luliconazole is an imidazole antifungal drug commonly used to treat dermatophytic infections like tinea pedis, tinea cruris, and tinea corporis. This research aimed to synthesize a transferosomal gel incorporating luliconazole for external applications. The thin film hydration method was employed to prepare luliconazole-loaded transferosomes using lecithin and tween 80 at varying concentrations. The transferosomes were characterized regarding particle size and entrapment efficiency. Subsequently, these transferosomes were incorporated into a carbopol gel base and evaluated for drug content, pH, spreadability, viscosity, in vitro release profile, and antifungal efficacy. The results indicated that the synthesized luliconazole transferosomes exhibited high entrapment efficiencies of 74.45% and 92.75%, with particle sizes ranging from 60-200 nm. Scanning electron microscopy confirmed the formation of spherical vesicles. The in vitro release study demonstrated a negative correlation between entrapment efficiency and release rate. The formulated gel showed good antifungal efficacy.
Keywords: Luliconazole, transferosomes, gel formulation, antifungal

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Abstract ID: ICCSHIP-2025/A-033

Development and Validation of Rp-Hplc Method for Estimation of Dapagliflozin in Solid Dosage Form

Surwase Mohini shivaji1
Dayanand College of Pharmacy, Latur – 413512, Maharashtra, India
*Email: mohinisurwase2@gmail.com

Abstract: Dapaglificzin Dapagliflozin are Active pharmaceutical al ingredient ingredient mostly used in the treatment of TYPE- -2 Diabetes Mellitus. An efficient and simple HPLC method has been developed and validated for the determination of Dapagliflozin in solid dosage form. The Mobile phase used for the chromatographic runs consisted of Sodium Acetate Buffer PH 4.5 THF Methanol (30:10:60). The Separation was achieved on Agilent STC-C18 Drug peaks were separated and detected by a UV detector at 223nm. The method has been validated according to ICH (Q2 R1) quidelines with respect to system suitability, specificity, precision, accuracy and range, robustness. The flow rate was 8 min. All the validation parameters were were found within the acceptable range.
Keywords: Dapagliflozin. RP-HPLC method validation.

Abstract ID: ICCSHIP-2025/A-034

Cinnamon Oil Offers Highly Efficient Alternative to Cedar Wood Oil for Microscopy Applications

Karale Mahesh[1], More Rahul[1], Bhete Shveta[1], Kamble Kajal[1]
[1]Department of Microbiology, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA
*Email: karale.mahesh@gmail.com

Abstract: Research into microscopy oils is an understudied area of biological research. Immersion oil enhances a microscope's resolving power by replacing the air gap between the immersion objective lens and the cover glass with a medium of high refractive index, thus reducing light refraction. While light refraction is generally not noticeable with lower magnification objective lenses (4x, 10x, 40x), it becomes significant when using a 100x objective with a dry lens. Reducing light refraction allows more light from the microscope slide to pass through the narrow diameter of the high-power objective. In microscopy, increased light translates to clearer, crisper images. By filling the air gap with a substance like immersion oil, which has a refractive index similar to the glass slide, more light is directed through the objective, resulting in a clearer image. Cedar wood oil is commonly used in microscopy. This study demonstrates that cinnamon oil can serve as a highly effective replacement. Experiments revealed that cinnamon oil has a refractive index of 1.52, compared to 1.48 for cedar wood oil. This makes cinnamon oil a very efficient substitute. Furthermore, cinnamon oil is readily available worldwide and is less expensive than cedar wood oil.
Keywords: Cinnamon oil, Cedar wood oil, Microscopy, Refractive index, Resolving power.

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Abstract ID: ICCSHIP-2025/A-035

Application of Multicomponent Reaction for the Synthesis 7-Amino-2-(4-Chlorophenyl)-5-Phenyl-5H- [1, 3, 4] Thiadiazolo [3,2-a] Pyrimidine-6-Carbonitrile Derivative With Their Biological Activity.

Swapnil V. Navhate[1], Ashok R. Karad[2], Vijay N. Bhosale[3]*
[1]Dept. of Industrial Chemistry, Sanjeevanee Mahavidyalaya, Chapoli, Dist. Latur (M.S), India.
[2]Department of Chemistry, Mahatma Gandhi Mahavidyalaya, Ahmedpur, Dist. Latur (MS),
[3]PG Research Centre, Department of Chemistry, Yeshwant Mahavidyalaya, Nanded (MS), India.
*Email: svnavhate@gmail.com.karad.ashok@gmail.com, bhosalevn@rediffmail.com

Abstract: A green, mild, most efficient, eco-friendly and simple method has been developed for the synthesis of 7-amino-2-(4-chlorophenyl)-5-phenyl-5H- [1,3,4] thiadiazolo[3,2-a] pyrimidine-6-carbonitrile derivatives from one-pot three component cyclocondensation reactions of various aromatic aldehydes, Malononitrile and Chlorothiadiazol in DMF by using an efficient catalyst K2Co3. The synthesized 7-amino-2-(4-chlorophenyl)-5-phenyl-5H- [1,3,4] thiadiazolo[3,2-a] pyrimidine-6-carbonitrile were screened for their Anti-microbial activity. These newly synthesized compounds were assessed by their using various spectroscopic techniques like NMR, IR, Mass.
Keywords: Aromatic Aldehydes, Malononitrile, Chlorothiadiazol, K2Co3, MCRs.

Abstract ID: ICCSHIP-2025/A-036

Deciphering the Molecular Composition and Functional Properties of an Orange Pigment from Paracoccus Beibuensis SL2

Deepti D. Dhere[1], S. M. Dharmadhikari[2]
[1] Department of Microbiology, Dayanand Science College, Latur
Affiliated to-Swami Ramanand Teerth Marathwada University, Nanded
[2]Government College of Arts and Science, Aurangabad, (M.S), India
Affiliated to Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, (M.S.) India.
*Email: deepti.dhere@gmail.com

Abstract: Paracoccus beibuensis SL2, a halo-alkalotolerant bacterium isolated from the Lonar Crater, Buldhana, Maharashtra, India, was identified using conventional and advanced techniques. The 16S rRNA sequence was deposited in the NCBI GenBank under the accession number KY129665. Recent investigations focused on the extraction and purification of a bright orange pigment produced by P. beibuensis SL2. Comprehensive analyses were performed using spectrophotometry, chemical assays, thin-layer chromatography (TLC), Fourier-transform infrared (FT-IR) spectroscopy, and high-performance liquid chromatography (HPLC) to determine the pigment's chemical nature. The acetone-extracted pigment exhibited a maximum absorption peak at 480 nm with a single prominent peak and a broad shoulder region, characteristic of xanthophyll pigments. Chemical tests confirmed the presence of polyene groups in the pigment. TLC analysis revealed an RF value of 0.74, consistent with the standard carotenoid trans-astaxanthin, belonging to the xanthophyll group. FT-IR spectroscopy further corroborated the xanthophyll nature, displaying characteristic peaks at 1739 cm^{-1} (C=O), 3380 cm^{-1} (O-H), 1647 cm^{-1} (C=C), and 1349

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cm^{-1} (C-C). HPLC analysis identified a major peak at a retention time of 3 minutes, matching the retention time of standard trans-astaxanthin, confirming it as the principal component of the pigment. These findings demonstrate that the bright orange pigment produced by P. beibuensis SL2 is a carotenoid, primarily a xanthophyll pigment resembling astaxanthin. Given its structural and functional properties, this pigment holds significant potential as a natural colorant and a therapeutic molecule with considerable commercial value.

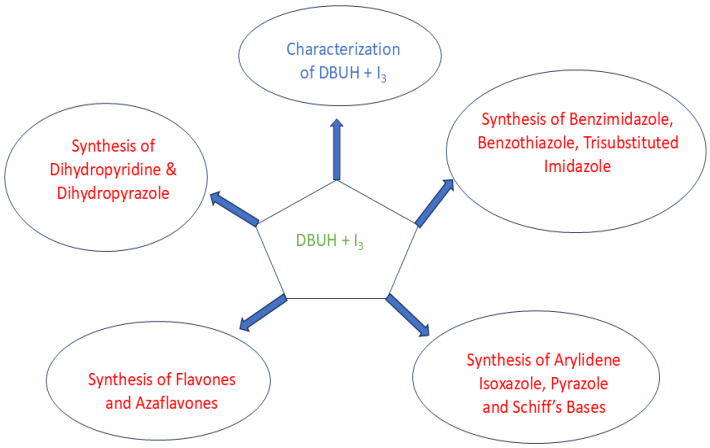
Keywords: Paracoccus beibuensis, Chemical analysis, TLC, FT-IR, HPLC.

Abstract ID: ICCSHIP-2025/A-037

DBUH+I3 as Novel Catalysis for Synthesis of Small Heterocyclic Molecules

Pramod Kulkarni*
Department of Chemistry & Post Graduate Research Center in Organic Chemistry
Hutatma Rajguru Mahavidyalaya, Rajgurunagar, Pune-410505
*Email: pramodskulkarni3@gmail.com

Abstract: We have synthesized and characterized the new amine-iodine complexes and their application as catalysts in forming diverse heterocyclic compounds. These complexes were identified through spectroscopic techniques, and physicochemical properties were studied. Among the various amine-iodine complexes screened, DBUHI3 was found as the most effective catalyst for promoting the synthesis of heterocycles, including benzimidazole, benzothiazole, 2,4,5-trisubstituted imidazole, arylidene isoxazole, arylidene pyrazole, heterocyclic Schiff's base, flavone, aza-flavone, dihydropyridine, and dihydropyrazole. Reactions were optimized in various solvents, leading to a process-optimized protocol. The structures of the synthesized compounds were confirmed using spectroscopic methods such as FT-IR, ^{1}H-NMR, ^{13}C-NMR, and HRMS. Key signals in these spectra validated the fundamental skeletons of the derivatives, with some confirmations reinforced by physical constants when compared to reported molecules. Overall, this work introduces new AmineH-Iodide complexes as efficient catalysts for organic transformations, supported by optimized protocols for high-efficiency synthesis.



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Abstract ID: ICCSHIP-2025/A-038

Characterization of Dye-Degrading Bacteria and Study of Their Kinetics

Parth Milind Kulkarni
Department of Chemistry, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA
*Email: parthkul2000@gmail.com

Abstract: Nowadays, the use of dyes is essential in numerous industries, as the color that attracts consumers has several serious issues, like health and environmental hazards, although some alternatives are not enough. As part of the new sustainable development, researchers have found that the concept of bioremediation shows that certain microbes can degrade the dye. Microbes have a specific enzyme that is responsible for the degradation and decolorization. This is a very innovative aspect of decolorization through microorganisms, if it may be applied to dye. The impact of environmental factors such as pH, temperature, and initial dye concentration was analyzed to determine the ideal conditions for achieving the highest levels of discoloration and degradation. The research involved using bacterial strains including PS1, PS2 &PS3. Among these strains, PS1 was selected for further study as it proved to be the most efficient decolorizer. The bacteria demonstrated greater discoloration under static conditions compared to when they were in shaken environments. For the decolorization process with PS1, a pH level of 7.0 was found to be the most effective, leading to successful decolorization.
Keywords: Dye degradation, Bacteria, Decolorization, Time factor, Kinetics.

Abstract ID: ICCSHIP-2025/A-039

Thermodynamic Study of Complexation of Tb (III) With Some Novel Schiff Bases in Mixed Solvent Media

Kuldeep Sakhare[1], Hansaraj Joshi[2]
[1]Department of Chemistry, Swa.Sawarkar College, Beed – 431122, Maharashtra, INDIA
[2]Department of Chemistry, Balbhim College, Beed – 431122, Maharashtra, INDIA
*Email: hansarajjoshi307@gmail.com

Abstract: The stability constant of Schiff base 4-hydroxy-3-(1-((5-phenyl)-1,3,4-thiadiazol-2 yl) imino) ethyl)-2H-chromen-2-one with metal ion Tb^{3+} using a pH metric titration technique in 80%(v/v) ethanol-water mixture at three different temperatures 25°C, 35°C & 45°C at an ionic strength of 0.1M $NaClO_4$ were studied. The Calvin-Bjerrum method as adopted by Irving-Rossotti has been employed to determine metal-ligand stability constant logK values. The thermodynamic parameters such as, Gibb's free energy change (ΔG), entropy change (ΔS) and enthalpy change (ΔH) associated with the complexation reactions were calculated.
Keywords: stability constant, Tb (III) metal ion, Schiff bases, pH metry, thermodynamic parameter etc.

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Abstract ID: ICCSHIP-2025/A-040

Microwave Assisted Synthesis of 2-Phenyl-2,3-Dihydro-1H Naphtho[1,2-e] [1,3] Oxazine Using Montmorillonite

Tukaram G Mundhe, Bhalchandra N Chate
Department of Chemistry, Sanjeevanee Mahavidyalaya Chapoli, Latur-413515 (M.S.), India
*Email: tgmundhe@gmail.com

Abstract: Oxazines are heterocyclic organic compounds containing one Oxygen and one Nitrogen atom in a cyclohexa-1,4-diene ring. Isomers [1,2],[1,3] and [1,4] exist depending on the relative position of the heteroatoms and relative position of the double bonds. 1,3-Oxazine compounds are widely used in medicines, organic dyes, and as synthetic intermediates. Present work describes the synthesis of 2-phenyl-2,3-dihydro-1H-naphtho[1,2-e] [1,3] oxazine using montmorillonite K10 catalyst under microwave irradiation. A multicomponent reaction between β-naphthol, formaldehyde and aniline in presence of montmorillonite K10 under microwave irradiation produces 2-phenyl-2,3-dihydro-1H-naphtho[1,2-e] [1,3] oxazine.
Keywords: Oxazine, montmorillonite, microwave irradiation

Abstract ID: ICCSHIP-2025/A-041

Environmentally Benign Synthesis of Isoxazolone Derivatives Using Lemon Juice Under Ultrasonic Conditions.

Vilas Vane[1], Ramesh Mokal[2], Gopinath Shirole[2], Suresh Jadhavar[1]
[1]Department of Chemistry, Yogeshwari Mahavidyalaya, Ambajogai - 431517 (MS), India.
[2]Department of Chemistry, A.S.C. College, Rahata, Ahmednagar - 423107 (MS), India
*Email: vilasvane@gmail.com

Abstract: Researchers reported a novel, solvent-free synthetic methodology for preparing Isoxazolone derivatives via the ultrasonic-assisted reaction of aryl aldehydes, ethyl acetoacetate (EAAC), and hydroxylamine in lemon juice. This approach is a natural acid-catalyzed multi-component reaction in an aqueous medium with excellent yields. Ultrasonic radiation condition helps, reaction rates are greatly accelerated and efficiency increases, allowing for quick synthesis with little energy input. This eco-friendly method reduces pollution in the environment by eliminating hazardous chemical solvents. Isoxazolone derivatives exhibit a broad spectrum of biological activities, including antimicrobial, anti-inflammatory, and anticancer properties, and are valuable for pharmaceutical and medicinal development

Keywords: Ultrasonic synthesis, Eco-friendly, Isoxazolone, Lemon Juice, Ethyl acetoacetate,

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Abstract ID: ICCSHIP-2025/A-042

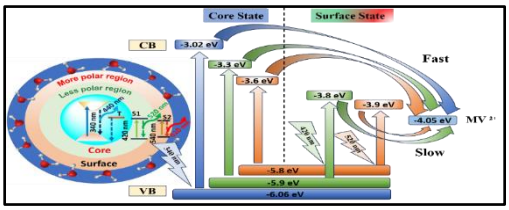
Ultrafast Insights into Electron Transfer Dynamics in Carbon Dots Reveal Heterogeneous Surface and Core States

Umarfaruk S. Sayyad, Somen Mondal*[a]

[a] Institute of Chemical Technology, Mumbai, Marathwada Campus, Jalna, Maharashtra 431203, India

*Email: sayyad.sab97@gmail.com

Abstract: Designing carbon dots (C-Dots) with precisely controlled optical properties has long posed challenges due to their intricate fluorescence and excitation-dependent emission characteristics. In this study, we synthesized three distinct types of C-Dots (blue, green, and red-emitting) using identical starting materials through hydrothermal methods, followed by separation using silica column chromatography. Despite differences in excitation wavelengths, all purified C-Dots exhibited uniform emission maxima and shared a particle size of approximately 4 nm, along with an interplanar spacing of about 0.21 nm. Our investigation into carrier dynamics revealed that graphitic nitrogen in the core, along with oxygen-containing functional groups on the surface, predominantly influence their emission properties. Further examination of the heterogeneity of these C-Dots, utilizing steady-state and time-resolved fluorescence, as well as ultrafast transient absorption spectroscopy, demonstrated that the core state has a significantly stronger electron transfer (ET) ability than the surface state, which is restricted by the oxygen-containing surface groups acting as electron scavengers. Additionally, our study indicated that both the graphitic nitrogen in the core and the oxygen groups on the surface contribute to the distinct electron transfer behavior observed in the C-Dots. These insights offer valuable guidance for the design of metal-free, light-harvesting systems and could facilitate the development of advanced C-Dot-based architectures with tailored properties.\



Abstract ID: ICCSHIP-2025/A-043

Studies on the Thalloids and Associated Mycorrhizae from Mahabaleshwar

Kashid J. K. Mule Y. B.

Shriman Bhausaheb Zadbuke Mahavidyalaya, Barshi

*Email: kashidjayaram@gmail.com

Abstract: Endomycorrhizae fungi indicate symbiotic relationship with plants. Frequently it forms abundant sports in soil. Biological characteristics of thallod liverwort Targionia hypophylla were analysed. Total seven fungal genera reported with Chaetomium sp. and Glomus sp.

Keywords: Endomycorrhizae, Thalloid, Biological characteristics.

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Abstract ID: ICCSHIP-2025/A-044

Synthesis and Biological Evaluation of Some Heterocyclic Compounds

Komal Doifode*, Dr. Shailaja Jadhav
PES's Modern College of Pharmacy Nigdi, Pune
*Email: komaldoifode775@gmail.com

Abstract:7-azaindoles shows lot of biological activities such as analgesic, anticancer, Rho-kinase inhibitor, Thrombin inhibitor, Antibacterial activity etc. A series of four 7-azaindole derivatives 6a-6d were synthesized and evaluated for antimicrobial activity. The compound 6a and 6d have shown excellent activity and 6c have shown equal potency as that of standard drug Azithromycin against gram negative bacteria (P. aeuginosa).
Keywords: Analgesic, Anticancer, Antibacterial, Antifungal, And Heterocyclic.

Abstract ID: ICCSHIP-2025/A-045

Nanomaterials for Supercapacitor Application

Kunale R.A.
Kai. Rasika Mahavidyalaya Deoni, Dis. Latur 413519, M.S., India
*Email: physicskrmd@gmail.com

Abstract: With the rapid global population growth, escalating environmental challenges, and the increasing reliance on energy-consuming devices, the development of efficient and sustainable energy storage solutions has become a critical area of research. As energy demands continue to rise, there is a significant push toward creating advanced, environment-friendly, and low-cost energy storage devices that can meet the needs of both modern society and the planet. Among the various types of energy storage technologies, hybrid supercapacitors have gained considerable attention due to their impressive combination of high energy density, high power density, fast charge/discharge capabilities, and exceptional cyclic stability. Nanostructured electrodes, such as porous carbon, conductive polymers, and metal oxide-based materials, are widely investigated for their high surface area, tuneable morphology, and superior conductivity. Here in this study we studied the development of binary polymeric nanocomposite consisting of $Ni_{0.5}Cu_{0.5}Fe_2O_4$ ferrite and Polyaniline (PANI) synthesized via in-situ polymerization of aniline monomer for high-performance supercapacitor applications. To investigate the structural and morphological properties of the as-synthesized NMF/PANI nanocomposites, we employed X-ray diffraction (XRD). The electrochemical performance of the pure ferrite and binary NMF/PANI nanocomposite was assessed using Cyclic Voltammetry (CV). At a current density of 1 A g^{-1}, the binary NMF/PANI nanocomposite exhibited a maximum specific capacitance of 215 F g^{-1}. These results suggest that the binary NMF/PANI nanocomposite is a promising candidate for use in high-performance supercapacitors.

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Abstract ID: ICCSHIP-2025/A-046

Formulation and Evaluation of Herbal hair Oil

Kunale R.A , A. G. Manjrekar*, S. S. Borkar, Dr. J. R. Baheti.
Department of Pharmaceutics, Rashtrasant Tukadoji Maharaj Nagpur University, Amravati Road, Gokulpeth, Nagpur -440033,MS, India
*Email: ashwinimanjarekar18@gmail.com

Abstract: Pharmacogonosy is the study of crude drugs, natural products obtained from plants, animals, or minerals, used in compound formulations. Ayurveda is the "science of life" and uses herbs in healthcare. Cosmetics are substances used to clean, beautify, or alter appearance without affecting the body's structure or functions. Hair is a protein fiber that develops from follicles within the dermis. Hair care products are applied topically to the scalp and hair, including detergents, conditioners, nutrient-rich ingredients, hair colorants, growth promoters, and anti-dandruff. This study aims to formulate and evaluate a polyherbal hair oil that promotes hair growth, smoothness, and vital nutrients. Various plant materials were collected for the preparation of the herbal oil. The formulated oil provides nourishing values to hair, preventing damage, loss, and dull hair while promoting growth.

Abstract ID: ICCSHIP-2025/A-047

Synthesis and Bio-Evaluation of New 1, 2, 3-Triazole Incorporated Polyhydroacridines as Antioxidant Agent

Ashruba B. Dannea[1], Jaiprakash N. Sangshetti[2], Bapurao B. Shingate[3]*
[1]Department of Chemistry, Balbhim Arts, Science and Commerce College Beed 431122, Maharashtra, India
[2]Y. B. Chavan College of Pharmacy, Dr. Rafiq Zakaria Campus, Chhatrapati Sambhajinagar 431001, Maharashtra, India
[3]Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar 431 004, Maharashtra, India
*Email: bapushingate@gmail.com

Abstract: The increasing impact of click chemistry in the field of medicinal chemistry and drug discovery. The concept of “click chemistry” was coined by Sharpless, i.e. copper-catalyzed 1,3-dipolar cycloaddition reaction of azides and alkynes which were very selective, high yielding and wide in scope. Hence, in recent years click chemistry has emerged as a fast and powerful approach to the synthesis of novel compounds. Polyhydroacridines and their derivatives are an important class of bioactive molecules in the pharmaceutical field. We were encouraged to combine 1,2,3-triazole pharmacophore unit with polyhydroacridine in a single molecular framework by using molecular hybridization approach. The newly synthesized compounds were characterized by IR, 1H-NMR, 13C-NMR and Mass spectral analysis. The synthesized 1,2,3-triazole incorporated polyhydroacridines was evaluated for their antioxidant activity and it showed excellent antioxidant activity. **Keywords:** 1, 2, 3-Triazole; Polyhydroacridine; Click chemistry, Antioxidant activity; Molecular hybridization.

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Abstract ID: ICCSHIP-2025/A-048

Formulation and Evaluation of Hair Conditioner by Using Okra Gel & Flaxseed Gel

P.V. Rathod*, Dr. A. Deshpande, Dr. J. R. Baheti
Department of Pharmaceutics, Rashtrasant Tukadoji Maharaj Nagpur University, Amravati Road, Gokulpeth, Nagpur -440033, MS, India
*Email: rathodpratiksha79@gmail.com

Abstract: Preparing hair conditioner is essential for silky, preventative hair. Okra gel and flaxseed extract are two examples of natural components used to make herbal hair conditioners, which are safe to use. Okra gel is a multifunctional hair care product that helps to maintain moisture, thicken hair, add gloss, and support healthy scalp function. Flaxseed hair conditioner, which is high in omega-3 fatty acids, accelerates hair growth and offers nourishment, while okra, which is rich in vitamins and minerals, supports hair strength, development, and growth. Both components are gel-like textures that strengthen hair and help lock in moisture, avoiding breaking. In addition to being natural and safe, herbal hair conditioners smooth, shine, and support healthy hair. By lowering friction between hair strands, hair conditioners make brushing easier.

Abstract ID: ICCSHIP-2025/A-049

Formulation & Evaluation of Rapid Dispersible Tablet by Using Different Concentration of Superdisintegrant & Its Comparsion with Marketed Preparation

R. B. Lohkare*, Dr. M. C. Gunde, Dr. J. R. Baheti
Department of Pharmaceutics, Rashtrasant Tukadoji Maharaj Nagpur University, Amravati Road, Gokulpeth, Nagpur -440033, MS, India
*Email: reshmalohkare7@gmail.com

Abstract: The present work focuses on formulation and evaluation of Aspirin Rapid Dispersible tablets by using different concentration of superdisintegrant i.e. Sodium Starch Glycolate (SSG) by direct compression method and comparison with commercially available Marketed preparation. The main objective was to enhance patient compliance. The available marketed preparation tablet takes at least 1minute to disperse. The main focus was to make Rapid Dispersible Tablets in such way that it may disperse within fraction of seconds. Formulations were evaluated and compared with Marketed Preparations. We have formulated Aspirin Tablets in different A1,A2,A3 and A4 batches containing Sodium Starch Glycolate 8% , 10% , 12% , 14% respectively. It was observed that by using low concentration of Superdisintegrant,it takes more time to disperse and with increase in its concentration it disperses rapidly. As per the results obtained, it was found that the formulation batch No A3 having concentration 12% of SSG was found to be similar with the marketed Preparation with special reference to dispersion time. Formulation batch No A4 having concentration 14% of SSG was found to be having dispersion time very less in comparison with the marketed preparations and which was found to be very beneficial to patient as it disperse rapidly and gives faster effect as compare to marketed tablet.

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Abstract ID: ICCSHIP-2025/A-050

Simultaneous Estimation of Glucosamine and Chondroitin Sulfate from Various Pharmaceutical Dosage Forms by Using a Stability Indicating Green Chemistry Analytical Methodology

Vijaykumar S. More,[1] Shrikant V. Kulkarni[2]

[1]Department of Chemistry, Kai.Rasika Mahavidyalaya Deoni, Dist.-Latur -413519, (M.S.), India

[2]Sava Healthcare Limited, Research Centre, Block D1, Plot no. 17/6, MIDC, Chinchwad, Pune-411019, (M.S.), India.

*Email: vijaymore@gmail.com

Abstract: Design and development of analytical methods with environment friendly reagents and solvents is the need of the hour for labs engaged in analytical services. Every year thousands of chemical and pharmaceutical laboratories worldwide are generating tones of toxic chemical wastage causing environmental pollution thereby endangering the human existence. The objective of this study was to develop and validate a sensitive, stability-indicating, accurate and precise green chemistry RP-HPLC method with RI detector for the simultaneous quantitation of glucosamine and chondroitin sulfate from various pharmaceutical dosage forms. Complete separation of both the actives was achieved in isocratic mode by using Hypersil BDS Phenyl (250 x 4.6 mm, 5µm) HPLC column. Purified water as a diluent and phosphoric acid buffer pH 2.5 was used as a mobile phase at a flow rate of 0.2 mL/min. The column temperature was maintained at 40°C. Both the molecules being non-chromophoric in nature, refractive index (RI) detector was used for detection.The method was found to be linear within the range of 5 - 770 µg/mL with r value 1.0000. The limit of quantification (LOQ) was set at 5µg /mL for both the actives which is lowest amongst the reported methods. The recovery for glucosamine was found to be 98.7% to 101.9% with 0.10 to 1.04 % RSD and 98.2% to 100.4% with 0.21 to 0.73 % RSD for chondroitin sulfate at different recovery levels with less than 2.0% inter and intraday precision. The developed method is successfully validated as per ICH guidelines. The method is stability indicating, sensitive and economical. Hence, it can be successfully used for the routine analysis of commercial batches of these combination products.

Abstract ID: ICCSHIP-2025/A-051

Zinc Sulphamate Catalyzed Eco-friendly Synthesis of Furanoquinoline Derivatives.

Mantosh Bhimashankar Swami*

*Mahatma Basweshwar Mahavidyalay, Latur, Maharashtra.

*Email: mantoshswami123@gmail.com

Abstract: Ecofriendly and efficient synthesis of furanoquinoline derivatives from aniline, substituted benzaldehyde and dihydrofuran using zinc sulphamate. Zinc sulphamate possesses Lewis's acidity and finds various catalytic applications with efficiency. The present methodology describes an efficient, ecofriendly and clean synthesis of furanoquinoline derivatives using catalytic amount of zinc sulphamate in ethanol: water at ambient temperature. The screening of solvent, catalytic amount and temperature was studied in detail, as a result 10 mol % of catalyst showed 100% conversion with 90% yield of furanoquinoline derivatives in water ethanol medium at

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ambient temperature. In addition, various biologically significant furanoquinoline derivatives was prepared under optimized condition with good yield. The significance of this present protocol is high yield, low cost, easy work up-procedure.

Keywords: Eco-friendly synthesis, efficient synthesis, Furanoquinoline derivatives, Zinc sulphamate

Abstract ID: ICCSHIP-2025/A-052

Formulation and Evaluation of Nanogel for the Treatment of Antifungal Disease

Nivrutti Kotsulwar, Mayur Upade
Channabasweshwar Pharmacy College (Degree) Kava Road, Basweshwar Chowk, Latur-413512
*Email: - nivruttikotsulwar2050@gmail.com

Abstract: Nanogels represent a cutting-edge nanotechnology-based platform for the delivery of antifungal agents, offering significant advantages such as enhanced drug solubility, controlled release, and targeted delivery. This study investigates the formulation and evaluation of a nanogel developed specifically for the treatment of antifungal diseases. The nanogel was synthesized using a biocompatible polymer matrix, optimized for critical parameters including encapsulation efficiency, particle size, and drug loading. Antifungal agents such as fluconazole and itraconazole were effectively incorporated into the nanogel, ensuring stability and sustained drug release. The nanogel was characterized using advanced analytical techniques, including dynamic light scattering (DLS) for particle size distribution, scanning electron microscopy (SEM) for morphological analysis, and Fourier-transform infrared spectroscopy (FTIR) to evaluate chemical compatibility. In vitro drug release studies demonstrated a controlled release profile, enhancing therapeutic efficacy and reducing side effects. Antifungal activity was assessed through microbiological assays against clinically significant strains, including Candida albicans and Aspergillus Niger, revealing substantial inhibition zones compared to conventional formulations. Furthermore, cytotoxicity assessments conducted on human keratinocyte cell lines confirmed the nanogel's favourable safety profile. These findings highlight the potential of this nanogel system to transform antifungal therapy by improving drug bioavailability, reducing systemic toxicity, and enhancing patient compliance. Future investigations will focus on clinical translation and scalability of the formulation to facilitate its widespread adoption in medical practice.

Keywords: Nanogel, Antifungal Diseases, Targeted Drug Delivery, Sustained Release, Topical Therapeutics, Fungal infections, Controlled drug release, Topical therapeutic system, Enhanced penetration, Nanotechnology, Localized therapeutic action.

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Abstract ID: ICCSHIP-2025/A-053

The Potential of Custard Apple Seed Extract in Managing Powdery Mildew of Custard Apple: A Natural Approach to Disease Control

Mitali Dattatraya Sonkamble
Dayanand College of Pharmacy, Latur.
*Email: - nivruttikotsulwar2050@gmail.com

Abstract: Powdery mildew, caused by fungal pathogens such as Oidium species, significantly affects custard apple (Annona squamosa) by reducing yield and fruit quality. The excessive use of chemical fungicides to control this disease can lead to environmental harm and fungicide resistance. This study investigates the antifungal potential of custard apple seed extracts as a natural and sustainable alternative to manage powdery mildew. Phytochemical screening of the extracts revealed the presence of alkaloids, flavonoids, and phenolic compounds, which exhibit strong antifungal properties. Laboratory and greenhouse trials demonstrated that methanolic extracts were particularly effective in reducing fungal growth and disease severity on infected custard apple plants. These findings suggest that custard apple seed extracts could serve as an eco-friendly solution for managing powdery mildew, promoting sustainable agricultural practices.
Keywords: Powdery mildew, custard apple, Annona squamosa, seed extract, bio-fungicide, sustainable agriculture.

Abstract ID: ICCSHIP-2025/A-054

Formulation and Evaluation of In-Situ Gel Containing Anti-Fungal Drug for Vaginitis

Mr. Rutik B. Wadje, Prof. Dr. Nagoba S.N.
Department of Pharmaceutics, Channabasweshwar Pharmacy College (Degree), Latur- 413512, Maharashtra, INDIA.
*Email: - rutikwadjepatil@gmail.com

Abstract: The objective of this study was to formulate and evaluate in-situ vaginal gels containing an antifungal drug. These systems rely on polymers that undergo sol-to-gel phase transition in response to changes in specific physicochemical parameters, such as pH. The formulations were evaluated for several key characteristics, including gelling capacity, viscosity, gel strength, microbiological properties, and in-vitro drug release. In this study, gellan gum(0.1–0.75%w/v) was used in combination with sodium carboxymethylcellulose to create a gel system that prolongs the release of the antifungal drug. Gels are increasingly used in drug delivery systems for their ability to provide controlled and prolonged drug release. The drug content, appearance, and pH of the formulations were all found to be within acceptable ranges, indicating good formulation stability,Viscosity measurements revealed that the sols exhibited viscosities ranging from 0.005 to 0.085 Ps, while the gel forms showed a significantly higher viscosity of 16 Ps.The formulations exhibited pseudoplastic flow behavior with thixotropic properties, indicating the ability to adapt the mechanical stress during application.The gel strength, as measured by a texture analyzer, was found to be up to 6.5 g. In vitro release studies demonstrated that the optimized formulations were capable of releasing the antifungal drug over a period of 360 minutes, providing a controlled drug delivery profile. These in-situ vaginal gels are expected to improve drug administration at the site of infection, reducing the frequency of application and enhancing patient compliance.
Keywords: In-situgels, controlledrelease, gellangum, sodiumcarboxy-methylcelluose.

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Abstract ID: ICCSHIP-2025/A-055

Extraction, Isolation and Characterization of Alkaloids with Anti-Gout Potential from Ardisia solanacea

Kalyani Munde*, .Jyotsna Chopade
Dr. D.Y. Patil College of Pharmacy, Akurdi, Pune
*Email: - mundekalyani75@gmail.com

Abstract: Gout is a clinical syndrome caused by the deposition of monosodium urate monohydrate crystals, which can trigger acute inflammatory responses in joints or accumulate in soft tissues without inducing inflammation. The increasing prevalence of gout highlights the need for alternative therapeutic approaches, particularly those based on natural products. The present study aims to extract, isolate, and characterize alkaloids from Ardisia solanacea, employing advanced techniques such as flash chromatography and High-Resolution Liquid Chromatography-Mass Spectrometry (HR-LCMS) for detailed profiling Fresh aerial parts of Ardisia solanacea were collected and air-dried. The powdered plant material was subjected to solvent extraction using methanol, ethanol, and chloroform in a Soxhlet extractor. The extracts were concentrated under reduced pressure, yielding crude alkaloid-rich fractions. The crude alkaloid extracts were purified using flash chromatography with gradient elution, employing silica gel as the stationary phase. The separation was monitored by Thin Layer Chromatography (TLC) to track fractions containing alkaloids. Alkaloid-rich fractions were collected and evaporated to dryness. The isolated alkaloids were analyzed using High-Resolution Liquid Chromatography-Mass Spectrometry (HR-LCMS) to obtain detailed molecular information. This study highlights the effective extraction and isolation of alkaloids from Ardisia solanacea, coupled with the use of advanced techniques like flash chromatography and HR-LCMS for detailed chemical analysis. The findings open avenues for further research into the pharmacological properties of these alkaloids, potentially contributing to the development of new therapeutic agents. Gout is a clinical syndrome caused by the deposition of monosodium urate monohydrate crystals, which can trigger acute inflammatory responses in joints or accumulate in soft tissues without inducing inflammation. The increasing prevalence of gout highlights the need for alternative therapeutic approaches, particularly those based on natural products.

Keywords: HRLC-MS, Flash Chromatography.Alkaloid, Anti-Gout,Ardisia Solanacea

Abstract ID: ICCSHIP-2025/A-056

Green Nanoparticles as Emerging Tools in the Treatment of Breast Cancer: A Comprehensive Review

Shaikh Alfiya Gaffar, Sayed Nishat Munawar
Dayanand College of Pharmacy, Latur
*Email: - alfiyashaikh07508@gmail.com

Abstract: Breast cancer remains one of the leading causes of cancer-related mortality in women worldwide, leading to the urgent need for innovative approaches to diagnosis and treatment. Green nanoparticles, synthesized through environmentally friendly methods using plant extracts or

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biological agents, have emerged as promising candidates in breast cancer therapy due to their unique properties that enhance their potential for biocompatibility, low toxicity, and multifunctional properties. This review explores the various types of green nanoparticles, including metallic (gold, silver, copper) and non-metallic nanoparticles (carbon-based, polymeric), highlighting their mechanisms of action in breast cancer treatment. The article also covers their potential as drug delivery systems, imaging agents, and hyperthermia treatment. Moreover, it examines the synergistic effects of green nanoparticles with conventional therapies such as chemotherapy, radiotherapy, and targeted therapies. The challenges of large-scale synthesis, stability, and regulatory approval are discussed, alongside future perspectives in clinical applications. Additionally, these nanoparticles can serve as efficient carriers for gene therapies or siRNA delivery to silence oncogenes associated with breast cancer progression. Despite their promising potential, challenges such as variability in synthesis, optimization of drug loading, and safety concerns remain. Overall, green nanoparticles present a promising, sustainable alternative in the fight against breast cancer, offering enhanced therapeutic efficacy and reduced side effects compared to traditional treatments. This review delves into the current state of nanoparticle research, its applications in breast cancer therapy and diagnosis, and the obstacles that must be overcome for clinical integration.
Keywords: Green chemistry, Breast cancer, Nanoparticles, Metallic Nanoparticles.

Abstract ID: ICCSHIP-2025/A-057

Synthesis of $MgFe_2O_3$ Nanoparticles via the Chemical Co-Precipitation route: XRD, FTIR, and VSM Characterization

[1]Shankar Dhanraj Birajdar, [2]Ravindra C. Alange
[1]Department of Physics and Electronics, Dayanand Science College, Latur – 413 512, (M.S.), India
[2]Department of Physics and Electronics, Shri Madhavrao Patil Mahavidyalaya, Murum-413605
*Email: - drshankarbirajdar@gmail.com

Abstract: Magnesium ferrite ($MgFe_2O_4$) nanoparticles were successfully synthesized using a simple co-precipitation method. The structural properties of the synthesized nanoparticles were investigated using X-ray diffraction (XRD), which confirmed the formation of a single-phase spinel ferrite structure with high crystallinity. The average crystallite size was calculated to be approximately 22 nm using Scherrer's formula. The presence of metal-oxygen vibrations at tetrahedral (581 cm^{-1}) and octahedral (432 cm^{-1}) sites in the ferrite structure was confirmed by FTIR results. The M–H loop of $MgFe_2O_4$ was recorded using a Vibrating Sample Magnetometer (VSM), and magnetic parameters, including saturation magnetization (Ms), coercivity (Hc), and retentivity (Mr), were derived from the VSM data

Keywords: Nanoparticles, Magnetic, XRD

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Abstract ID: ICCSHIP-2025/A-058

Synthesis of Various 1, 5-Benzodiazepines Derivatives and Studied Their Antimicrobial Activity

Kendre Madhav Marotirao
Department of Chemistry, Shri Sant Gadge Maharaj Mahavidyalaya, loha Tq. Loha Dist. Nanded-431708 Maharashtra, INDIA
*Email: - madhavkendre72@gmail.com

Abstract: In recent time millions of heterocyclic compounds were synthesized due to their specific activity are employed in the treatment of many infectious diseases. Their use in the treatment is attributed to their inherent toxicity of various pathogens. Among a wide range of heterocyclic compounds that have been explored for the development of pharmaceutically important molecules. Most of the heterocyclic compounds are well known due to their biological importance. Out of these 1, 5-benzodiazepines are important seven member heterocyclic molecules which represent a variety of biological activities. A series of-2, 4-(substituted-phenyl)-2, 3-dihydro-1H-1, 5-benzodiazepine derivatives (2a-j) have been synthesized by the treatment of 1-(substituted-2-hydroxy-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (1a-j) with 4-methyl-ortho-phenylene diamine and few drops of piperidine using 20 ml methanol as a solvent was refluxed for 4 hrs. Then glacial acetic acid (5 ml) was added to the reaction mixture and refluxing was continued for 2 hrs, after completion of reaction (checked by TLC). The reaction mixture was left overnight at room temperature. In 70-80% yield with high purity, characterization of compounds was confirmed by the IR, 1H NMR and mass spectral analysis. All these newly synthesized compounds were evaluated for theirantibacterial activity against four different pathogens such as Escherichia coli, Salmonella typhi, Staphylococcus aureus and Bacillus subtilis and antifungal activity against Aspergillus niger, Penicillium chrysogenum, Fusarium moneliforme and Aspergillus flavus, using Penicillin and Greseofulvin using Peniciline and Greseofulvin as standard drugs by agar cup method and Poison plate method, respectively.

Keywords: 2-Hydroxy-chalcones, ortho-phenylene diamine, 1, 5-Benzodiazepines, Antimicrobial activity

Abstract ID: ICCSHIP-2025/A-059

Drug Design and Development

Wattamwar Vishranti Pradeep
Dayanand College of Pharmacy, Latur – 413512, Maharashtra, India
*Email: - vishrantiwattamwar@gmail.com

Abstract: Carbon nanotubes (CNTs) have received increasing attention in biomedical fields because of their unique structures and properties, including high aspect ratios, large surface areas, rich surface chemical functionalities, and size stability on the nanoscale. Particularly, they are attractive as carriers and mediators for cancer therapy. Through appropriate functionalization, CNTs have been used as nanocarriers for anticancer drugs including doxorubicin, camptothecin, carboplatin, cisplatin, paclitaxel, Pt (II), and Pt (IV), and genes including plasmid DNA, small-in- terfering RNA, oligonucleotides, and RNA/DNA aptamers. CNTs can also deliver proteins and immunotherapy

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components.

Using combinations of light energy, they have also been applied as mediators for photothermal therapy and photodynamic therapy to directly destroy cancer cells without severely damaging normal tissue. If limitations such as a long-term cytotoxicity in the body, lack of size uniformity during the synthetic process, loading deviations for drug- CNT complexes, and release controllability at the target point are overcome, CNTs will become one of the strongest tools that are available for various other biomedical fields as well as for cancer therapy.

Keywords: Carbon nanotubes, Cancer, Therapy, Carrier, Mediator

Abstract ID: ICCSHIP-2025/A-060

Investigating Splicing Events and RNA Stabilization in FBN1 Gene Mutation for Marfan Syndrome Therapy

Prapti Jadhav, Supriya Jadhav
Dayanand College of Pharmacy, Latur
*Email: sagarjadhav20091@gmail.com

Abstract: Marfan syndrome is a genetic disorder caused by mutations in the FBN1 gene, which encodes fibrillin-1, a key extracellular matrix protein. These mutations often disrupt normal splicing of FBN1 mRNA, resulting in a truncated, dysfunctional protein that leads to the clinical manifestations of the disease. Our research aims to elucidate the splicing events influenced by these mutations and to explore potential therapeutic strategies. Specifically, we are focusing on the secondary structure of both the wild-type and mutant FBN1 RNA to understand how mutation-induced splicing defects contribute to disease. To counteract the effects of the mutation, we are investigating the conformational change between wild type and mutated FBN1 RNA. By using RNA SHAPE study, we hypothesize there is change in conformation of mutated RNA due to the presence of splice site mutation and it hamper or alter the splicing event, leading to the production of truncated or improper fibrillin-1 protein. This approach could responsible for the development of Marfan syndrome, potentially mitigating the symptoms caused by the mutation. Our findings could open the door to RNA-based therapeutic interventions for Marfan syndrome and similar diseases.

Abstract ID: ICCSHIP-2025/A-061

Benign Chemistry of Dispiro-Hydroquinolines via a One-Pot Multicomponent Reaction

Pawde Shubhangi S., D. B. Muley
Research centre and P G Department of Chemistry, Shivaji Mahavidyalaya, Udgir
*Email: - muleydb@gmail.com

Abstract: A protocol has been developed for the synthesis of dispiro [tetrahydroquinoline-bis(5,5-dimethylcyclohexane-1,3-dione] derivatives via a one-pot multicomponent reaction of aryl amines, aromatic aldehydes, and Dimidone . Silica supported perchloric acid ($HClO_4$-SiO_2) was used as an efficient catalyst for the synthesis of dispiro[tetrahydroquinoline-bis(5,5-dimethylcyclohexane-1,3-dione] derivatives. The products were successfully synthesized in solvent free conditions and room temperature along with the suggested mechanism through combination of domino Knoevenagel, Michael, and Diels–Alder reactions. The remarkable advantages offered by this method are

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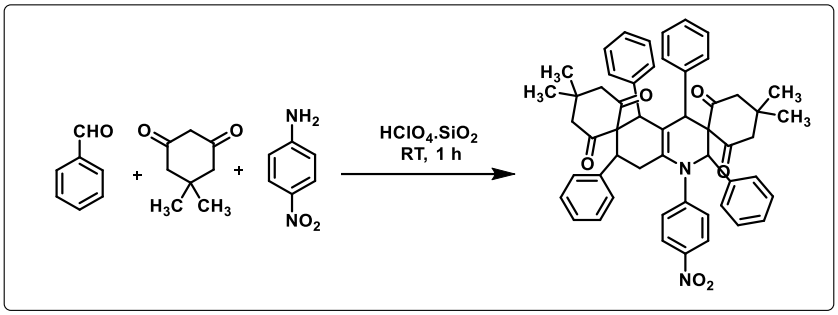
inexpensive catalyst, good yields, simple and easy work-up procedure. The products have been characterized by IR, mass, 1H NMR, 13C NMR spectroscopy, and elemental analysis. The compounds synthesized were examined through biological activities.

Keywords: Aromatic aldehydes, Aromatic amines, Dimidone, Dispiro compounds

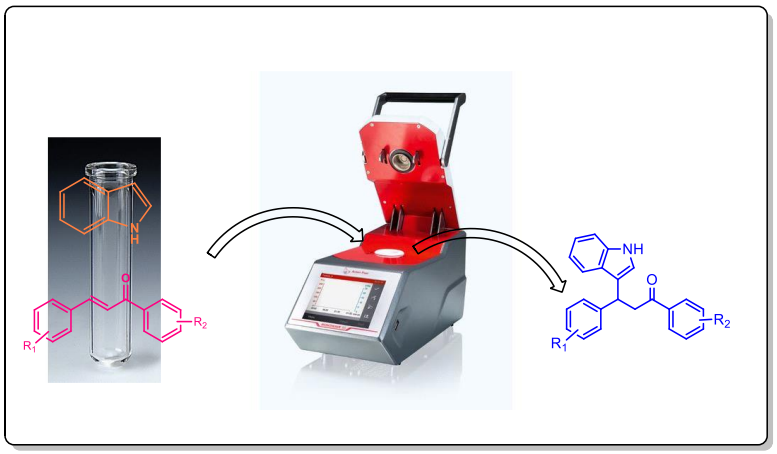


Abstract ID: ICCSHIP-2025/A-062

Microwave Assisted Synthesis of 3-(1H-Indol-3-yl)-1, 3 diphenylpropan-1-one) Derivatives

Neha Deshmukh, Omkar Pawar, Mahadevi Kamble, S. S. Mahurkar
Department of Chemistry, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA
*Email: - shreyas.mahurkar@gmail.com

Abstract: In this study, we report a microwave assisted approach for the synthesis of 3-(1H-indol-3-yl)-1, 3-diphenylpropan-1-one) derivatives using catalyst. The reaction involves the Michael addition of indole to chalcone. The structure of the synthesized products was confirmed using FT-IR, 1H NMR, and 13C NMR spectroscopy. This study focuses on the rapid synthesis of these derivatives using microwave irradiation, which offers advantages such as reduced reaction times, improved yields, and enhanced selectivity compared to conventional heating methods



Keywords: Microwave, Chalcone, Indole, Michael addition

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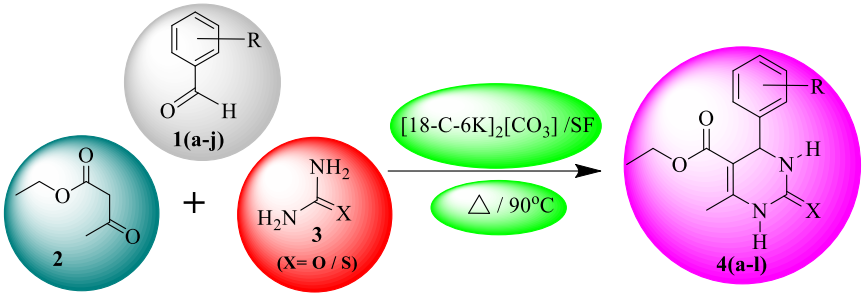
Abstract ID: ICCSHIP-2025/A-063

18-Crown-6 Complex Cation Ionic Liquid as an Efficient Catalyst for the Synthesis of 3,4-Dihydropyrimidin-2(1H)-one Under Solvent Free Condition.

Ramesh Mokal,[1] Gopinath Shirole,[2] Vilas Vane,[1] Suresh Jadhavar[1]*
[1]Department of Chemistry, Yogeshwari Mahavidyalaya, Ambajogai, Beed (MS), India
[2]Department of Chemistry, SSRI's, A.S.C. College, Rahata, Ahmednagar (MS), India
*Email: - rameshmokal1981@gmail.com

Abstract: An efficient method has been developed for the Biginelli synthesis of 3,4-dihydropyrimidin-2(1H)-one analogues by three component reaction of aryl aldehyde, acetoacetic ester and urea/thiourea under the influence of catalytic amount of Crown Ether Complex Cation Ionic Liquid (CECIL) $[18\text{-C-6K}]_2[CO_3]$ under solvent free reaction. This crucial Biginelli transformation in combination with $[18\text{-C-6K}]_2[CO_3]$ catalytic material is offered many advantages for the world of synthetic organic chemistry such as eco-friendly approach, simple thermal condition, easy workup procedure, without use of toxic organic solvents, short reaction time and good yield of the products.

Graphical Abstract: Synthesis of 3,4-dihydropyrimidin-2(1H)-one derivatives using $[18\text{-C-6K}]_2[CO_3]$



Keywords: Crown Ether Complex Cation Ionic Liquid (CECIL), $[18\text{-C-6K}]_2[CO_3]$, Biginelli reaction, Pyrimidinedione, Solvent free reaction etc.

Abstract ID: ICCSHIP-2025/A-064

Phytochemical Screening, In Silico Studies and Several Novel Pharmacological Activities of Plant Extracts of Monoon Longifolium

Rutuja Magar*, Seema Gaikawad*, Mrudul Dange, Dr.S.R.Butle
School of Pharmacy, Swami Ramanand Teerth Marathwada University, Nanded-431606
*Email: - rutujamagar2050@gmail.com

Abstract: Exploring the Antiparasitic Potential of Monoon longifolium Leaf Extracts against Trichomonas vaginalis and Neisseria gonorrhoeae. Trichomoniasis (Trichomonas vaginalis) and gonorrhea (Neisseria gonorrhoeae) are major sexually transmitted infections with increasing drug resistance to standard treatments like Metronidazole and Ceftriaxone, necessitating alternative therapies.This study investigates the antiparasitic properties of Monoon longifolium leaf extracts prepared using six solvents (methanol, water, glacial acetic acid, ethyl acetate, toluene, and hexane). Phytochemical analysis revealed bioactive compounds such as flavonoids, polyphenols, and

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alkaloids. Soxhlet extraction yielded the highest extractive efficiency with ethyl acetate (7.92%) and glacial acetic acid (10.6%). High-resolution LC-MS identified 63 compounds in the ethyl acetate extract, including 3-O-trans-Feruloyleuscaphic Acid and Ganosporelactone A. Molecular docking showed strong binding affinities of 3-O-trans-Feruloyleuscaphic Acid (-14.7) against T. vaginalis and Goyaglycoside A (-15.1) against N. gonorrhoeae. In vitro, ethyl acetate extracts exhibited significant inhibition (35 mm zone) for both pathogens, outperforming standard antibiotics. These results highlight Monoon longifolium extracts, particularly ethyl acetate and glacial acetic acid, as promising candidates for alternative treatments, warranting further research.
Keywords: Trichomonas vaginalis, Neisseria gonorrhoeae, HRLCMS analysis, Molecular docking.

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An Analysis of the Water Characteristics of Beaches In and Around Mumbai Region, Maharashtra, India

Sanjay Shukla, Vipul Purohit
Department of Chemistry, Thakur College, Kandivali(E), Mumbai-400101;
Affiliated to University of Mumbai
*Email: - vipulpurohit7@gmail.com

Abstract: Beaches are a place to unwind in a city like Mumbai, where people lead hectic and stressful lives. Aside from this, the beaches' water serves a number of residential and commercial uses, including the fishing industry, which supports the country's economy. The state of the water has gotten worse as a result of human activity and the administration's careless attitude. Monitoring the water quality is crucial to improving this concerning situation. The current project entails the scientific collection of water from the several beaches in the Mumbai area, including Juhu, Gorai, and Manori Island. In order to determine how different seasonal variations affected the water quality, water samples were collected every three months. The estimate of several physico-chemical parameters that affect water quality is part of the current investigation. Electrical conductivity, total hardness, COD, DO, pH, color, alkalinity, and TDS are among the different parameters being examined. Chemical and instrumental approaches were used to test these characteristics. Different levels of contamination in different water bodies are the subject of the investigation. According to the data collected, some parameters were found to be beyond the WHO-established limit, putting aquatic life in jeopardy. In order to help the relevant authorities, take corrective action to enhance the quality of the water on these beaches, the current study takes a relative approach to the water quality from various locations.
Keywords: Aquatic life, chemical and instrumental procedures, physico-chemical parameters, and the fishing industry.

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Abstract ID: ICCSHIP-2025/A-066

Rational of Chromen-2-One Based Hybrid Molecules as Potential Anti-Tubercular Agents and Their Docking for Mtb.

Siddheshwar B. Lonari, Anil S. Kirdant*, Suresh C. Jadhavar*
Department of Chemistry, Yogeshwari Mahavidyalay Ambajogai, Beed– 431517 (M.S) India.
Email: - sidlonari24@gmail.com, dr.askirdant@gmail.com

Abstract: Tuberculosis (TB) remains a critical global health challenge, as identified by the World Health Organization (WHO), which names it the world's leading infectious killer. Caused by Mycobacterium tuberculosis, TB primarily affects the lungs, leading to symptoms such as chronic cough, weight loss, and fatigue, though it can also impact other organs, including the brain, kidneys, and spine. Transmission occurs when individuals inhale droplets containing the bacteria, allowing it to reach the alveoli after passing through the respiratory tract. Currently, the FDA-approved medications for TB treatment include rifampin, isoniazid, pyrazinamide, and ethambutol. This study aims to develop a naturally occurring compound through synthetic chemistry, targeting TB with modifications at side chains to achieve lower IC50 values compared to existing drugs. For the Synthesized of substituted amide Derivatives (3a – 3j) to achieve this, a library of amides was synthesized and coupled with a chromen molecule is Compound 4a – 4 j. the final synthesized compound was subjected to pharmacokinetic studies and molecular docking to evaluate its efficacy.

Keywords: Tuberculosis, Anticancer, Antidiabetic activities, Umbelliferone (7-Hydroxy 4 Methyl coumarin), Amides.

Abstract ID: ICCSHIP-2025/A-067

Vipera Nikolskii Venom Used in SARS-CoV

Tikambare Saraswati Vijayanand, Kshirsagar Satyasham Prashant
Dayanand College of Pharmacy, Latur – 413512, Maharashtra, India
*Email: - saraswatitikambare@gmail.com

Abstract: Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), the causative agent responsible for the coronavirus disease-2019(Covid-19). SARS-CoV-19 was identified in December 2019 in the Chinese city, Wuhan.Coronavirus disease is a pulmonary disease, In which local direct vascular and endothelial injury occur in the lungs and other organs leads to clot formation and angiopathy,leads to thrombosis in the pulmonary arteries (Pulmonary embolism) and arteries of brain(stroke). In severe Covid-19 patients' pulmonary embolism and stroke has been reported in 20-30% and 3-5% respectively. Peptides or antithrombotic proteins may help in covid-19. It binds to enzymes angiotensin converting enzyme 2 act as receptor, improvement in vascular function occur, it make the blood vessels relax. Vipera nikolskii venom boon against covid-19.

Keywords: SARS-CoV-2, Pulmonary embolism, Stroke, Angiotensin converting enzyme-2, Vipera nikolskii venom

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Ultrasonic Studies of Plasticizer Solutions

Smita S. Kharkale-Bhuyar
Department of Chemistry, Shri Lemdeo Patil Mahavidyalaya, Mandhal, Kuhi, Nagpur, Maharashtra, India
*Email: - smitakharkale2013@gmail.com

Abstract: Current works on the equilibrium and active properties of polymer solutions obtained from ultrasonic measurement. The dissolved states of polymer in solutions, the amount of solvated solvent and hydrated water, and the degree of counterion binding of polyelectrolytes were discussed on the basis of the sound velocity measurement at a few MHz. the ultrasonic relaxation processes in the frequency range from several hundred KHz to a few hundred MHz were interpreted by the local segmental motion of polymer in solution. The ultrasonic degradation of plasticizer in solutions is briefly discussed.
Keywords: Ultrasonic degradation, Ultrasonic velocity, Ultrasonic relaxation processes.

Abstract ID: ICCSHIP-2025/A-069

Coconut Shell Derived Carbon Dots and its Application as Nanocatalyst in Heterocyclic Compound Synthesis

Rakesh Kumar Sonkar[1], Archana Asartkar[2], Prasanna Sharma[1]*, Prashant Kumdale[3]
[1]Amity University, Raipur, Chhattisgarh, India
[2]Govt.Nagarjuna P.G. College of Science, Raipur, Chhattisgarh, India
[3]Department of Chemistry Shivneri College Shirur Anantpal, Latur, MS, India
*Email: - rakeshsonkar90@gmail.com, asatkar@gmail.com, pkpk7389@gmail.com

Abstract: Since heterocyclic compounds are widely used in materials science, agrochemicals, and pharmaceuticals, their synthesis is essential to organic chemistry. Because of their large surface area, adaptable functionality, and eco-friendliness, carbon dots (or CDs) have become a promising class of nanocatalysts. The creation of carbon dot nanocatalysts using coconut shell biomass—a plentiful and renewable waste resource—is the main goal of this work. In order to improve their catalytic performance, the CDs were surface functionalized after being created using a simple pyrolysis and hydrothermal method. The structural and morphological characteristics of the CDs were investigated using sophisticated characterization methods such as Raman spectroscopy, FTIR, XRD, and TEM. During the production of several heterocyclic compounds, including pyrimidine, pyrazole, and others, the resultant carbon dots demonstrated remarkable catalytic efficiency.
Keywords: carbon dots, coconut shell, nanocatalyst, heterocyclic compounds, green chemistry, biomass-derived materials

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Abstract ID: ICCSHIP-2025/A-070

Design, Molecular Docking Study of Some New N-€-Phenylmethylidene-1H-indole-3-Carbohydrazide Derivatives as Tyrosinase Inhibitors and In vitro Evaluation of Their Anti-tyrosinase and Antioxidant Activities.

Sujata Datt
Department of Pharmaceutical Chemistry, Channabasweshwar Pharmacy College (Degree), Latur – 413 512, Maharashtra, INDIA
*Email: - sujatadatt12@gmail.com.

Abstract: Tyrosinase and its related proteins are responsible for pigmentation disorders & inhibiting Tyrosinase is an established strategy to treat hyperpigmentation. The Indole-scaffold can be effective inhibitors of Tyrosinase activity. A novel series of some 1H-Indole-3-carbohydrazide derivatives are designed to study their inhibitory activity against tyrosinase. Two proteins i.e.(PDB ID-5MBL & PDB ID-2Y9X) are selected for docking studies Swiss ADME properties were calculated and we were found that designed derivatives were followed the lipinski rule of 5.Indole carbohydrazide derivatives showed the 0 violance after checking with Swiss ADME, it means they follows the lipinski rule of 5.
Keywords: Tyrosinase inhibitor, Indole-3-carbohydrazide derivatives, protein-2Y9X, 5MBL.

Abstract ID: ICCSHIP-2025/A-071

Anti-arthritic Activity of Passiflora Incarnate

Suraj Allishe
Dr. D. Y. Patil College of pharmacy Akurdi pune
*Email: - surajallishe144@gmail.com

Abstract: Rheumatoid arthritis RA is an autoimmune condition with a suspected etiology, prevalence of 0.5% or more in the population and can cause disability through joint degeneration through synovitis inflammation and progressive cartilage and bone degeneration leading to slow steady rigidity or immobility. Herbal products are natural products that have in-borne medication that can heal a certain disease or ailments of arthritis symptoms. In the present study Anti-arthritic activity of Passiflora incarnate leaves using methanolic extract was performed. Extraction was done by maceration process, further suitable dose was prepared as per acute oral toxicity and given to animals (Rats). **Keywords:** Rheumatoid Arthritis, Herbal drugs, Passiflora incarnate to treat arthritis.

Abstract ID: ICCSHIP-2025/A-072

Synthesis and Antimicrobial Activity of 2-(2-Arylamino-4 Phenyl Thiazol-5-yl)-5-Substituted Benzofuran Derivatives

Suryawanshi V. S.[1] Chavan J. L[2], Mugle Y. G[1].
[1]Dept. of Chemistry, P.G. and Research Centre, Shri Chhatrapati Shivaji College, Omerga
[2]API, R and D Centre, Emcure Pharmaceuticals Limited, Hinjewadi, Pune
*Email: - surajallishe144@gmail.com

Abstract: A series of 2-(2-arylamino-4-phenylthiazol-5-yl)-5-substituted benzofuran derivatives were synthesized from 1-aryl-3-(N-phenylbenzimidoyl)thiourea and 2-(2-bromoacetyl) -5-

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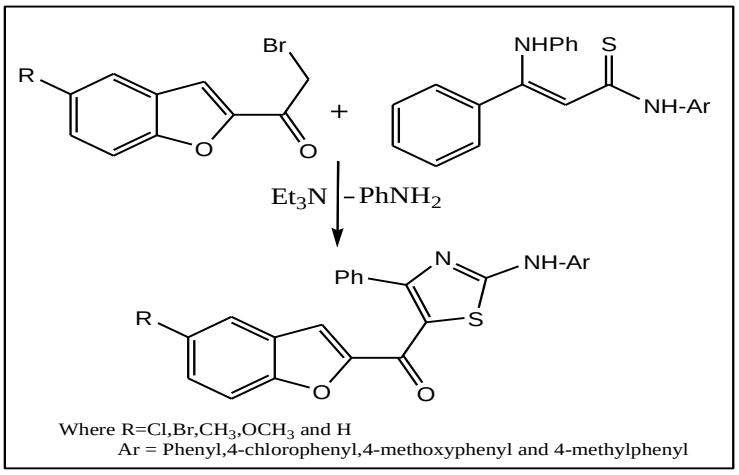
substituted benzofuran in the presence of triethylamine. Their structure was established on the basis of IR,1H NMR and Mass spectral techniques. The entire newly synthesized compounds were screened for their antifungal and antibacterial potential. All the compounds showed low to moderate activity against the microorganisms tested.

Reaction Scheme:



Where R=Cl,Br,CH_3,OCH_3 and H
Ar = Phenyl,4-chlorophenyl,4-methoxyphenyl and 4-methylphenyl

Abstract ID: ICCSHIP-2025/A-073

Realization of Self-Cleaning Properties on Textile Surface Using Nanotech Material

Vidya N. Aiwale[1], .N. S. Korde[2]
[1]Department of Chemistry, Yogeshwari Mahavidaylaya, Ambajogai Dist.Beed-431517
[2]Department of Chemistry, Dayanand Science College, Latur-413512,Maharashtra,India
*Email: - vidya.namdas01@gmail.com

Abstract: Water and soil repellency has been one of the major targets for fiber and textiles scientists and manufacturers for centuries. Combinations of new materials for fiber production with a variety of surface treatments have been developed to reach the condition of limited wettability. Developing a new concept or applications are use of bio-photocatalyst, Single and Binary Systems of metal oxides, nanocomposites, etc, for photo catalytic degradation of organic pollutants. Existences of such pollutants are serious hazard to flora & fauna and leading to the destruction of ecosystem. Recently, photo degradation of various synthetic dyes has been studied in terms of their absorbance and the reduction of oxygen content by changes in the concentration of the dye. The advantages that make photo catalytic techniques superior to traditional methods are the ability to remove contaminates in the range of ppb, no generation of polycyclic compounds, higher speed, and lower cost. Taking this into account, the research exploration will encompass development of newer heterogeneous binary systems for photo-catalytic degradation of colored pollutants.

Keywords: Nanoparticles, photodegradation, dyes, photocatalyst

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Abstract ID: ICCSHIP-2025/A-074

Investigating the Spectroscopic, Photoluminescence, Electrochemical Impedance and Thermal Characteristics of Cerium Oxide (CeO2) Nano Rods

Tikeshwar[1], Archana Asatkar*[1], Prashant Kumdale[2]

[1]Department of Chemistry, Govt. Nagarjuna P.G. College of Science Raipur, Dist. Raipur -492010 India

[1]*Department of Chemistry, Govt. Nagarjuna P.G. College of Science Chhattisgarh-492010 MS, India

[2]Department of Chemistry, Shivneri College ShirurAnantpal Dist. Latur-413544 MS, India

*Email: - asatkar@gmail.com

Abstract: Cerium dioxide (CeO_2) or Ceria nano rods had been produced within the modern-day paintings, the usage of the chemical precipitation method. X-ray diffraction, Fourier transform infrared spectroscopy, X-ray photoelectron spectroscopy scanning electron microscopy UV photoluminescence and electrochemical impedance spectroscopy, thermo gravimetric and differential thermal analyses (TG/DTA) were used to assess the fabric characteristics of the produced samples. The XRD effects screen that the CeO_2 nano rods crystallized into the cubic fluorite crystal device. Micro-strain dislocation density, advantage length and cellular quantity of the samples have been assessed. XPS examination became carried out to verify the chemical states of the constituent elements in CeO_2 nano rods. FTIR spectral analysis changed into used to investigate chemical bonds and molecular vibrations in CeO_2 nano rods. SEM analysis turned into used to look at the grain structure of CeO_2 nano rods. UV–visible spectroscopy decided the CeO_2 optical absorption traits, band gap, and strength. PL examines and CIE-chromaticity mapping had been used to research the light-emitting traits of the CeO_2 nano rods. The EIS method turned into applied to have a look at the impedance nature of CeO_2 nano rods. TGA/DTA investigations have been performed to locate the thermal characteristics of CeO_2 nano rods. The take a look at findings indicate the usefulness of CeO_2 nano rods as electrodes and optoelectronic substances

Keywords: CeO_2, XRD, SEM, PL, FTIR, XPS, EIS, etc.

Abstract ID: ICCSHIP-2025/A-075

Impact of Fe Doping on Mn_3O_4 Thin Films: Structural, Optical, and Morphological Insights

Priyanka Biradar[1], Dr. Vijendra Chaudhari[1]

Thin Films and Materials Science Research Laboratory, Department of Physics, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA

*Email: - pya.biradar@gmail.com, vijendra333@gmail.com

Abstract: This study presents the synthesis and characterization of pure and 5% Fe-doped manganese oxide (Mn_3O_4) thin films prepared via spray pyrolysis. The thin films were deposited on pre-cleaned glass substrates heated to a 400°C temperature. The structural, optical, and morphological properties of the synthesized thin films were systematically studied using X-ray

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diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and field-emission scanning electron microscopy (FE-SEM). XRD analysis confirmed the formation of tetragonal Hausmannite Mn_3O_4 with high crystallinity. The introduction of Fe ions led to slight shifts in peak positions and changes in peak intensities, indicating successful in-corporation of Fe into the Mn_3O_4 lattice. UV-Vis spectroscopy measurements revealed a decrease in the optical band gap from 2.6 eV for pure $Mn_3O_4$to 2.2eV as the 5% Fe doping concentration. FE-SEM images demonstrated uniform, densely p acked granular nanostructure thin films. The Fe-doped films exhibited slight changes in surface morphology compared to pure Mn_3O_4 films.

Keywords: Mn_3O_4 thin films, spray pyrolysis, XRD, UV-Vis spectroscopy, FE-SEM, band gap.

Abstract ID: ICCSHIP-2025/A-076

Synthesis and Spectral Characterization of Schiff Base Ligands Derived from Dehydroacetic Acid (DHA)

More A. L.[1]*, Chougule A. M.[2]

[1]Department of Chemistry, BV'S Matoshri Bayabai Shripatrao Kadam Mahavidyalaya, Kadegaon, Dist- Sangli. (MS) -415304, India.

[2]Department of Industrial Chemistry, Dayanand Science College, Latur. (MS) -413512, India.

*Email: - amolchem1@rediffmail.com, annaraochougule@gmail.com

Abstract: The reaction of primary amine with an aldehyde or ketone under specific condition to form Schiff Bases [1]. Schiff base a significant class of organic compound with a (>C = N—) functional group, have gained significant attention in chemistry due to their remarkable synthesis methods, diverse properties, and wide-ranging applications. There is great interest in developing a wide range of applications in organic synthesis [2]. It is well known for its various synthetic and physiological properties. In this study, a series of Schiff bases were synthesized by the condensation of 3-acetyl-4-hydroxy-6-methyl-2H-pyran-2-one (DHA) with various 5-(substituted phenyl)-1, 3, 4-thiadiazol-2-amine. The chemical structures of synthesized Schiff bases were characterized using various analytical techniques such as IR spectra, UV/VIS spectrophotometry, proton nuclear magnetic resonance (1H-NMR), elemental analysis, and melting point determination and mass spectrometry.

Keywords: Schiff Bases, synthesis, thiadiazol, physiological

Abstract ID: ICCSHIP-2025/A-077

Formulation and Evaluation of Polyherbal Hair Serum for Treatment of Pediculosis Capitis.

Gopika Dinesh Nawgaje, Hemant Devrao Sarnaik, Ajay Raju Thakare

School of Pharmacy, S.R.T.M.U. Nanded

*Email: - gopikanawgaje2001@gmail.com, hemantsarnaik35@gmail.com, ajaythakare1745@gmail.com

Abstract: The aim and objective of the present study are to formulate and evaluate Anti-lice polyherbal hair serum for treatment of pediculosis capitis using Annona squamosa leaves, Citrus Limon fruit, Citrus Limon leaves and Cinnamomum tamala leaves extract. The antilice activity of

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the prepared formulation was tested using MTT assay and they exhibited a good Anti-lice activity. The prepared formulation was evaluated for various physicochemical parameters for which good characteristics were observed. The easy availability of plants and their effectiveness helps manufacturers with cost effective benefits and with less or no side effects.

Abstract ID: ICCSHIP-2025/A-078

Comprehensive Analysis of Secondary Metabolites: Classification, Pharmacological Activities of Terpenoids, and HR LC-MS Profiling of Terpenoids in A. Solanaceae

Kunal Warwatkar*, Mrs.Jyotsna Chopade
Dr. D Y Patil college of pharmacy, Akurdi, Pune
*Email: - warwatkarkunal@gmail.com

Abstract: Secondary metabolites are crucial bioactive compounds synthesized by plants for defense, survival, and ecological interactions. A. solanaceae is a plant rich in secondary metabolites, including terpenoids, a structurally diverse class derived from isoprene units. Terpenoids exhibit a wide range of pharmacological activities, including anti-inflammatory, antimicrobial, anticancer, and antioxidant effects. High-resolution liquid chromatography-mass spectrometry (HR LC-MS) is a sensitive and precise technique used to profile these compounds, uncovering their therapeutic potential and significance in drug discovery. To classify secondary metabolites in A. solanaceae, investigate the pharmacological activities of terpenoids, and utilize HR LC-MS for comprehensive profiling to reveal their therapeutic potential.To conduct a comprehensive analysis of secondary metabolites with a specific focus on the classification and pharmacological activities of terpenoids, and to utilize high-resolution liquid chromatography-mass spectrometry (HR LC-MS) for profiling terpenoids in A. solanaceae, aiming to uncover their therapeutic potential and role in drug discovery.Phytochemical Profiling:HR LC-MS Analysis: Identification and quantification of terpenoids and other secondary metabolites using high-resolution liquid chromatography-mass spectrometry. Structural elucidation based on chromatographic retention times and spectral data. Diversity of Metabolites: A. solanaceae contains various secondary metabolites, predominantly terpenoids with complex structures. Pharmacological Activities: Terpenoids exhibited significant therapeutic activities, including anti-inflammatory, antimicrobial, anticancer, and antioxidant properties. HR LC-MS Profiling: High-resolution analysis identified unique terpenoid compounds, emphasizing their pharmacological importance and potential for drug development. A. solanaceae is a valuable source of bioactive terpenoids with significant therapeutic potential. The application of HR LC-MS enabled the precise profiling of these metabolites, supporting their role in traditional and modern medicine. Further studies focusing on the isolation, synthesis, and clinical evaluation of these terpenoids could pave the way for novel drug discoveries.

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Abstract ID: ICCSHIP-2025/A-079

Facile Hydrothermal Synthesis of Carbon Dots from Caesalpinia Crista L. Leaves and their Characterization

Rajesh Valvi[1], Anil Athare[1]*, Sushama Takate[2]
[1]Department of Chemistry, New Arts, Commerce and Science College, Shevgaon Dist. Ahmednagar, Maharashtra- 414502, India.
[1]*, [2]Department of Chemistry, New Arts, Commerce and Science College, Ahmednagar, Maharashtra- 414001 India.
*Email: - ltanilathare@gmail.com

Abstract: Plant-derived carbon dots (CDs) have attracted considerable attention due to their multifunctional surface, biocompatibility, low toxicity and multiple applications in medical and other fields. To provide the first report on CDs derived from CCL leaves and analyze their structural, morphological and spectroscopic properties.The present synthesis work utilizes the leaves of CCL to synthesize CDs through easy and simple hydrothermal method. The synthesized CDs were characterized using ultra violet-visible (UV-Vis), Fourier transform infrared (FT-IR) and Raman spectroscopy, in combination with X-ray diffraction (XRD), High resolution transmission emission microscope (HR-TEM) and elemental analysis.The UV-Vis spectra of CDs exhibits two maximum absorption peaks at 227.7 nm and 379.4 nm, while the FT-IR spectrum identifies a vibrational frequencies of bonds at 3350, 1712, 1620 and 1070 cm^{-1}. Raman spectroscopy shows the D and G bands are at 1354 cm^{-1} and 1594 cm^{-1}, respectively. The XRD analysis reveals prominent peaks at 28.3° and 40.5°, while the HR-TEM and selected area electron diffraction (SAED) images confirm the formation of quasi-spherical, uniformly distributed and amorphous CDs with an average particle size of 7.9 nm. Elemental analysis finding indicate that the carbon was predominant component followed by oxygen, hydrogen and nitrogen.The leaves of CCL can be used as a green precursor for the synthesis of CDs by hydrothermal methods with average size 7.9 nm and UV-Vis, FT-IR, Raman spectroscopy, XRD, HR-TEM and elemental analysis as fundamental characterization techniques.

Abstract ID: ICCSHIP-2025/A-080

Evaluation of Anti-ulcer Activity of Slippery elm bark Extract in Wister Rats

Sushil Ramrao Bhalerao
School of Pharmacy, Swami Ramanand Teerth Marathwada University, Nanded
*Email: - sushilbhalerao605@gmail.com

Abstract: Peptic ulcers are a prevalent and widespread health issue, free radicals production, a decline in mucosal defense's mechanism, or an increase in mucosal damaging elements is among the main causes. Slippery elm plant is known for its different phytoconstituents such as mucilage Uronic acid, Pentose, Hexose, Methyl Pentose (rhamnose, galactose). Others- Tannins, Oxalate acid, flavonoids, Phytosterols, Salicylic acid, capric acid, caprylic acid, decanoic acid. The most abundant and medically important, biochemical components of slippery elm are flavonoids, mucilage and tannins. Flavonoids have antiulcerogenic properties, tannins that display strong

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antioxidant activity nucleic acid formation can be influenced by free radicals generated during oxidative stress and protection against reactive oxygen species, several cellular processes, including lipid peroxidation, protein denaturation, carbohydrate and, so it was selected for evaluation of its anti-ulcer activity.

Keywords: Slippery elm, Auntiulcer, Ulcer index, Ranitidine

Abstract ID: ICCSHIP-2025/A-081

Design and Application of Nanostructured Metal-Organic Frameworks (MOFs) for Targeted Drug Delivery

Vaishnavi Jaykumar Budhe
School of Pharmacy, Swami Ramanand Teerth Marathwada University, Nanded
*Email: - budhevaishnavi1@gmail.com

Abstract: The integration of nanotechnology and material chemistry has revolutionized the field of targeted drug delivery, offering solutions for precision medicine with minimal side effects. Nanostructured metal-organic frameworks (MOFs) have emerged as a promising class of materials due to their high surface area, tunable pore size, and versatile chemical functionality. This poster explores the synthesis, characterization, and application of functionalized MOFs in delivering therapeutic agents with enhanced efficacy and specificity. A two-step synthesis approach was employed to fabricate MOFs with tailored pore environments suitable for encapsulating hydrophobic and hydrophilic drugs. Advanced characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), and dynamic light scattering (DLS), were used to confirm the structural integrity and uniform size distribution of the MOFs. Functionalization with biocompatible ligands and surface coatings was achieved to improve stability in physiological conditions and enable targeted delivery. The poster also presents results from in vitro and in vivo studies demonstrating the controlled release of anticancer drugs, reduced cytotoxicity to healthy cells, and enhanced uptake by tumor tissues due to receptor-mediated endocytosis. The incorporation of imaging agents into MOFs for theranostic applications highlights their potential for simultaneous diagnosis and therapy. This research underscores the potential of nanostructured MOFs in advancing the field of precision medicine and suggests directions for future work in scaling up production and exploring synergistic therapies.

Abstract ID: ICCSHIP-2025/A-082

Recent Progress in Synthesis, Structure and Biological Screening of Some Phenothiazine Derivatives

Balasaheb Deshmukh
Dept. of Chemistry, GVISH, Amravati, Maharashtra 444601
*Email: - drbalu02@gmail.com

Abstract: The phenothiazine nucleus is one of the most important and trusted heterocyclic rings, which is commonly found in natural products and medicinal agents. It was discovered during the 1940s, since many scientists found various newer derivatives and established their biological

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activities. The recently developed phenothiazine derivatives were exhibiting significant activities such as tranquillizer, antibacterial, antiparkinsonian, antifungal, anticancer, antiviral, anti-inflammatory, antihistaminic, anti-malarial, anti-filarial, trypanocidal, anticonvulsant, analgesic, immunosuppressive and multidrug resistance reversal properties. In the presented study, an attempt had been made to systematize the recent research finding of many newer phenothiazine derivatives including method of synthesis, structure and evaluated in vitro and in vivo promising biological activities and pharmacological properties. This review emphasizes the two decades of research work on newer synthesis, structure and biological activities of different phenothiazine derivatives.

Abstract ID: ICCSHIP-2025/A-083

Phytochemical Analysis, In Silico and In-vitro Study of Cynodon Dactylon Leaves Extract for Insecticidal Activity

Bandgar Prajakta Prakash
School of Pharmacy, SRTMU Nanded
*Email: - ddkale8548@gmail.com

Abstract: Cynodon dactylon, commonly known as Bermuda grass, is a versatile medicinal plant widely recognized for its phytochemical properties. This study focuses on the phytochemical analysis, in silico evaluation, and in vitro investigation of C. dactylon leaf extract for its potential insecticidal activity. The phytochemical screening revealed the presence of bioactive compounds such as flavonoids, alkaloids, tannins, and phenols, which are known for their pesticidal properties. Pass studies were performed to predict the insecticidal activity. In vitro assays further validated the insecticidal activity, showcasing significant mortality rates against selectedspecies. The study highlights the potential of C. dactylon as a sustainable source for the development of eco-friendly insecticides and emphasizes its importance in integrated pest management strategies.
Keywords: Cynodon dactylon, phytochemical analysis, Insecticidal activity, Eco-friendly insecticides, Integrated pest management

Abstract ID: ICCSHIP-2025/A-084

Green and Efficient Synthesis of Novel 8, 9-Dihydro-8, 8-Dimethyl-2, 5-Diphenyl - 5H –[1, 3, 4] Thiadiazolo [2, 3-b] Quinazolin-6-(7H)-One Derivatives

B. D. Kamale, S. D. Rakhe, S. S. Mahurkar, J. A. Angulwar
Department of chemistry, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA
*Email: - jaangulwar@gmail.com

Abstract: A green and efficient synthetic approach for the preparation of 8,9-dihydro-8,8-dimethyl-2,5-diphenyl-5H-[1,3,4]thiadiazolo[2,3-b]quinazolin-6(7H)-one derivatives is described. This synthesis proceeds via a one-pot, multi-component reaction (MCR) of 2-amino-5-phenyl 1, 3, 4-thiadiazole, aromatic aldehyde and dimedone in presence of ionic liquid under ultrasonic conditions. The synthesized compounds were characterized by various spectroscopic techniques, including NMR, IR, and mass spectra to confirm their structure and purity.
Keywords: Ultra-sonication, Aldehyde, dimedone, 2-amino-5-phenyl 1, 3 , 4-thiadiazole, ionic liquid

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Carbon Nanotubes: Applications in Pharmacy and Medicine

Mukhedkar Swanand Shrinivasrao[1], Deshmukh Jitendra Hanmantrao[2]
Department of Chemistry Shahir Annabhau Sathe Mahavidyalaya Mukhed.[1]
Department of Chemistry Mahatma Basweshwar Mahavidyalaya, Latur (MS)[2]
*Email: - jaangulwar@gmail.com

Abstract: Carbon nanotubes (CNTs) are allotropes of carbon, made of graphite and constructed in cylindrical tubes with nanometer in diameter and several millimeters in length.Because of their structural, mechanical, and electronic properties are due to their small size and mass, strong mechanical potency, and have high electrical and thermal conductivity. CNTs have been successfully applied in pharmacy and medicine due to their high surface area that is capable of adsorbing or conjugating with a wide variety of therapeutic and diagnostic agents (drugs, genes, vaccines, antibodies, biosensors, etc.It works as drug delivery directly into cells without metabolism by the body. Then CNTs have been useful in drug and gene therapies but also for tissue regeneration, biosensor diagnosis, enantiomer separation of chiral drugs, extraction and analysis of drugs and pollutants. Moreover, CNTs have been recently act as antioxidant. It also examines the pharmacokinetics, metabolism and toxicity of different forms of CNTs and discusses the perspectives, the advantages and the obstacles of this promising bio nanotechnology in the future.

Abstract ID: ICCSHIP-2025/A-086

Green Chemistry

Chate R. R., Reddy P. S., Tirpude H.A
Chemistry Department, PG students in Shivaji Mahavidyalya Udgir, (MH)-413517
*Email: - radhachate2017@gmail.com

Abstract: The object of Green Chemistry is the reduction of chemical pollutants flowing to the environment. The Chemistry and the Environmental Division has assumed Green Chemistry as one of its areas of interests, but one question to solve is where Green Chemistry should be placed within the context of Chemistry and Environment. The concept of Green Chemistry, as primarily conceived by Paul Anastas and John Warner, is commonly presented through the twelve principles of Green Chemistry. However, these twelve principles through fruits of a great intuition and common sense, do not a clear connection between aims, concepts, and related research areas of Green Chemistry. The Twelve unsolved questions are the object of the present article.

Keywords: Green Chemistry's Principles, Pharmaceuticals, Sustainable Chemistry

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In-Vitro Anthelmintic Activity on the Plumeria Rubra L.

Vijay Govind Pawar[1], Nitesh Nandkumar Chavan[2]
Nanded Pharmacy College, Nanded, Maharashtra, India
*Email: - chavannitesh5201@gmail.com

Abstract: The plant extract of plumeria rubra was used on fresh adult earthworms for determining anthelmintic activity. They were collected from wet soil and exposed to various concentrations of plant extract in a hydro-alcoholic medium. The amounts of plant extract at 40, 80, 120, 160, and 200 µg/ml were examined; a control group containing 40 µg/ml of albendazole was also examined. The duration of time it took for the worms to become paralyzed and die was used to express the results. The paralysis and death of earthworms were monitored over time. Additionally, the morphological changes and behavioral responses of the earthworms were recorded. This study aimed to investigate the anthelmintic activity of the extract against earthworms in vitro Plumeria rubra leaves including glycosides, flavonoids, and saponins.
Keywords: Plumeria rubra, Anthelmintic, Earthworm etc.

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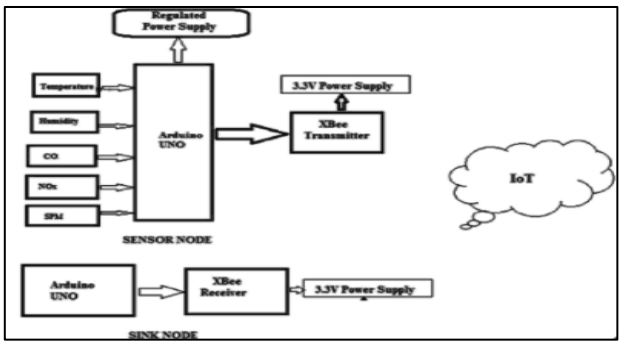
WSN and IoT based Smart Environment Monitoring Framework

T.H. Mujawar[1], R.B. Shinde[2]
[1]Department of Electronics, Dayanand Science College, Latur
[2]Department of Computer Science, Dayanand Science College, Latur
*Email: - m.tabbsum@gmail.com

Abstract: Technology advancements have led to a trend toward device downsizing, which necessitates the development of robust, low-powered, and costly sensors. As a result, Wireless Sensor Networks (WSN) have become important in a variety of applications, including environmental monitoring, industry, agriculture, and homes. An environment can be monitored and managed with the use of a wireless sensor network system. The proposed environment monitoring system detects temperature, humidity, CO, NOx, and suspended particulate matter (SPM). The Pollution Control Department's recommended traditional air quality monitoring technology is quite expensive. Typical gas sensors that are commercially available and integrated into a mote (Sensor Node). To create the measurements of sensing employed in the constructed network, a precise LabVIEW software is used. The Internet of Things (IoT) enables remote system monitoring.
Keywords: WSN, Co Sensor, NOx Sensor, LabVIEW and IoT etc.

Block Diagram:



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Abstract ID: ICCSHIP-2025/A-089

Recent advances in cytomegalovirus infection management in solid organ transplant recipients

Nikita Govind Murde, Sakshi Renukadas Maid
Dayanand College of Pharmacy, Latur
*Email: maidsakshi7@gmail.com

Abstract: Purpose of Review: Human cytomegalovirus (CMV) remains the most significant infectious complication following solid organ transplantation (SOT).Recent Findings: Universal prophylaxis and pre-emptive therapy are the most widely adopted strategies for the prevention of CMV disease globally. Prophylaxis using valganciclovir is the most common approach for CMV prevention; however, issues such as leukopenia and late-onset CMV disease after stopping prophylaxis necessitate the development of new strategies to prevent this complication. The use of assays that detect CMV-specific T cell-mediated immunity may help tailor the duration of antiviral prophylaxis after transplantation. Recently, letermovir has been approved for prophylaxis in kidney transplant recipients. Utilizing CMV-RNAemia alongside CMV-DNAemia in the viral surveillance of CMV infection provides accurate information on viral load kinetics, especially in patients receiving letermovir for prophylaxis or therapy. The emergence of refractory and resistant CMV infections remains a significant challenge, but the new treatment option maribavir is now available. This paper reviews the most recent advances in the prevention and treatment of CMV diseases in SOT recipients. The recent findings summarized in this paper may help optimize the prevention and treatment of CMV infection in SOT recipients.

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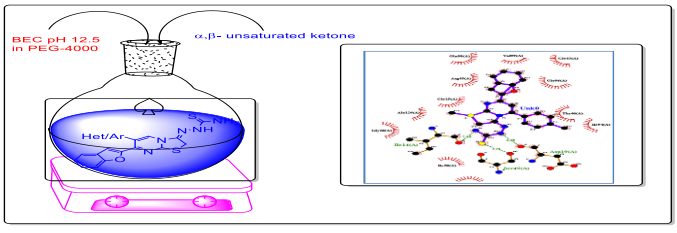
Abstract ID: ICCSHIP-2025/A-090

Design, Synthesis and Antituberculosis Activity of Thiazolo[3,2a] Pyrimidin-3 (8aH)-ylidene) Hydrazine Carbothioamide Derivatives

Milind V Gaikwad[1], Ashok P Acharya[2], Bhaskar S. Dawane[3]*
[1]Department of Chemistry, Dr. D. Y. Patil ACS College Pimpri, Pune, (M.S.), India
[2]Department of Chemistry, Mudhoji College, Phaltan, Satara (M.S.), India
[3]School of Chemical Sciences, Swami Ramanand Teerth Marathwada University, Nanded.(M.S.),
*Email: - milind.gaikwad@dypvp.edu.in

Abstract: We have designed series of novel (E)-2-(7- (benzofuran-2-yl)-6-phenyl-2H-thiazolo [3, 2-a] pyrimidin-3(8aH) ylidene) hydrazinecarbothioamide derivatives andsynthesized by combining benzofuran-2-yl)-6-phenyl-2H-thiazolo [3,2- a] pyrimidin-3(8aH)-one motif with hydrazine carbothioamide. The synthetic strategy adopted for the present protocol is supporting the green chemistry principals. The synthesized compounds are subjected for molecular docking with f 1dg5 enzyme. The compounds further evaluated for antitubercular activities. Amongst these synthesized compounds, the compounds7c, 7d, 7f, 7g, 7i, and 7jshows well to moderate antitubercular activities.
Keywords: PEG-400, Hydrazinocarbothoamide, molecular docking, Antitubercular activities



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Abstract ID: ICCSHIP-2025/A-091

Synthesized Polypyrrole (Ppy Nps) Nanocrystal Effect on Antimycobacterial, Cytotoxicity Performanance

Jivan Rameshrao Kote
Vishwasrao Naik Arts, Commerce and Baba Naik Science Mahavidyalaya,
Shirala, Dist- Sangali-415408.
*Email: - kotej2015@gmail.com

Abstract: Polypyrrole (Ppy Nps) are some of the most attractive nanomaterials because of their unusual physicochemical, mechanical, and electrical properties as well as their broad range of potential applications. The improvement of new resistant strains of antimycobacterial to current antibiotics has become a serious problem in public health administrative; therefore, there is a strong incentive to develop new Antimycobacterial agent [1].This makes current research in Anti TB agent nanomaterials particularly timely. Early studies indicated that the PolyNps size and surface area are important material characteristics from a toxicological perspective [2–5]. As the size of Ppy Nps decreases, the specific surface area increases, leading to increased opportunity for interaction and uptake by living cells. The Polypyrrole nanoparticles (Ppy Nps) we tested against three different Mycobacterium species like M.tuberculosis (MTCC-300), M.pheli (MTCC-1723), and M.avim (MTCC-1724). In contrast to Ppy Nps, where the direct interactions between NPs and bacteria were limited, Ppy Nps to three different strains enhanced Ppy Nps toxicity to cells and dramatically reduced cellular blood toxicity. Potential anti-oxidant agent Oxidative polymerization reaction Ppy Nps reduced the total number of living Mycobacterium strain. The PpyNps are characterization by XRD, SEM, TEM, FTIR,

Keywords: Polypyrrole (PpyNps), Antimycobacterial, Hemolytic assay, XRD, SEM, TEM, and FTIR.

Abstract ID: ICCSHIP-2025/A-092

Design and Green Synthesis of Some New 2-(4-phenylthiazol-2-yl) Phthalazin-1(2H)-One Derivatives by One Pot Multicomponent Approch

Pramod D. Jawale Patil
Department of Chemistry, Balbhim Arts, Scinece and Commerce College Beed. MS, India.
*Email: - pramodjawalepatil@gmail.com

Abstract: Sustainable chemistry basically addresses the integrated plan of chemical transformation and method to reduce the utilization and production of stuffs, harmful to the ecosystem and health of human being [1]. In this context , multiphase chemical transformation have lime lighted stellar, and are known as one-pot “multicomponent reaction” (MCRs) that must require more than three different or same substances, that leading to result simple or complex molecules, in which preferably consolidate most atoms or group of atoms from reactant [2]. However, one pot multiphase chemical transformation (MCTs) have been ingrained as a predominant pliers in combinatory synthetic organic chemistry as they are simplistic, productive, atom sustainability and accountable to controllable process [3]. In order to diverse application in multicomponent reactions

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(MCRs), it has been evolved as one of the divine tactics to gain the unavoidable requirement for development medicinally efficient thiazole derivatives and numerous biologically potent heterocycle. Based on the biologically active heterocycle thiazole, we successfully synthesized a series of some new aryl substituted 2-(4-phenylthiazol-2-yl) phthalazin-1(2H)-one derivatives (3a–3d). Herein we developed a mild and efficient protocol for the synthesis of aryl substituted 2-(4-phenylthiazol-2-yl) phthalazin-1(2H)-one derivatives by using Ethanol: Water solvent system for catalyst free method. 1H NMR, 13C NMR, ESI-HRMS, IR, element analysis, UV/Vis spectroscopy and fluorescence spectroscopy were performed to comprehensively characterize their chemical structures, spectral properties and stability.

Abstract ID: ICCSHIP-2025/A-093

In-Silico Methods for Drug Discovery: A Comprehensive Review Approch

Mitali Sonkamble, Ajit Giri, Shivkanta Puyed
Dayanand College of Pharmacy Latur
*Email: - puyedshivkanta@gmail.com

Abstract: In-silico methods have transformed the landscape of drug discovery, offering cost-effective and time-efficient approaches to identify potential drug candidates. This review highlights key computational methodologies, their applications, and challenges in modern drug discovery. We discuss molecular docking, virtual screening, quantitative structure-activity relationship (QSAR) modelling, molecular dynamics (MD) simulations, and machine learning (ML)-based approaches, emphasizing their integration into traditional workflows.

Abstract ID: ICCSHIP-2025/A-094

Nanorobotics

Sonali Govind Potdar, Jadhav Shruti Divakar
Dayanand College of Pharmacy, Latur
*Email: - drxsp25@gmail.com

Abstract: Nanorobotics is the technology of creating machines or robots at or close to the microscopic scale of a nanometer (10−9 meters). More specifically, nanorobotics refers to the still largely hypothetical nanotechnology engineering discipline of designing and building nanorobots, devices ranging in size from 0.1-10 micrometers and constructed of nanoscale or molecular components. As no artificial non-biological nanorobots have yet been created, they remain a hypothetical concept. The names nanobots, nanoids, nanites or nanomites have also been used to describe these hypothetical devices. Nanorobotics is an emerging, advanced and multidisciplinary field that calls for scientific and technical expertise of medical, pharmaceutical, bio-medical, engineering as well as other applied and basic scientists. Nanorobots differ from macro-world robots, specifically in their nano sized constructs. Assembly and realization of nanorobots depend on the principles of molecular nanotechnology and mechano-synthetic chemistry. Practically, these systems are nano-electromechanical devices that are capable to carry out pre-programmed functions in a reliable and accurate manner with the help of energy provided by a preinstalled nanomotor or

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nano-machine. Due to their small size and wide functional properties, nanorobots have created exceptional prospects in medical, biomedical and pharmaceutical applications. Although, no technology is available to construct artificial nanorobots, it is now possible to create nanorobots by using biological means. The review presents a brief discussion on basic nano-robotics and its possible applications in medical, biomedical and pharmaceutical research.

Keywords: Nanotechnology, Nanomedicine, Nanomachines, Nanomotors, Bionanorobots

Abstract ID: ICCSHIP-2025/A-095

Drug Design and Development

Dipmala .K.Borolkar, Ustad Saleha
Department Of Chemistry, Shivaji Mahavidyalaya Udgir, (MH)- 413517
*Email: - deepaborolkar09@gmail.com

Abstract: The Processes used by academic and industrial scientists to discover new drugs have recently experinced a true renaissance, with many new and exciting techniques being devleoped over the past 5-10 years alone. Drug design and discovery ,and research for new safe and will tolrated compounds,as well as the ineffectiveness of existing therapies , and societys insufficient Knowledge cocerning the prophylactics and pharmacotherapy of the most common diseases today, comprise a serious Challenge . This can influence not only the quality of human life, but also the health of whole societist, which became evident during Covid-19 pandemic. In general ,the process of drug development consists of three main stages : drug discovery ,preclinical development using cell-based and animal models/tests ,clinical trials on human and,finally forward moving toward the step of obtaining regulatory approval ,in order to market the potential drug.

Abstract ID: ICCSHIP-2025/A-096

Synthesis, In-Vivo Anti-Diabetic & Anticancer Activities and Molecular Modelling Studies of Tetrahydrobenzo[D]Thiazole Tethered Nicotinohydrazide Derivatives

Deshmukh Jitendra Hanmantrao
Department of Chemistry Mahatma Basweshwar Mahavidyalaya, Latur (MS) India
*Email: jhdeshmukh25@gmail.com

Abstract: The new thiazole-pyridine derivatives were synthesized by reaction of 4,4,7,7-tetra-methyl-4,5,6,7-tetrahydrobenzo[d]thiazol-2-amine with 6-chloronicotinate and by condensing with benzaldehydes and screened for their anti-diabetic activity by in vivo housing. All synthesized compounds resulted in reducing the glucose level when compared with reference standard drug glibenclamide. In specific, compound 7 exhibited significant activity in terms of fasting blood glucose level reduction. In addition, the in-silico binding studies of the potential compounds 11f and 11g with human PPAR-γ protein complexed with Retinoid X Receptor (RXR) alpha Nuclear Receptor showed good interactions when compared to the standard drug Rosiglitazone. The newly synthesized drugs may be potential anti-diabetic drugs with possible specific actions.

Keywords: Tetrahydrothiazole Pyridine hydrazide Anti-diabetic activity Molecular modeling.

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Abstract ID: ICCSHIP-2025/A-097

Design and Application of Nanostructured Metal-Organic Frameworks (MOFs) for Targeted Drug Delivery

Vaishnavi Jaykumar Budhe
School of pharmacy, Swami Ramanand Teerth Marathwada University Nanded
*Email: - budhevaishnavi1@gmail.com

Abstract: The integration of nanotechnology and material chemistry has revolutionized the field of targeted drug delivery, offering solutions for precision medicine with minimal side effects. Nanostructured metal-organic frameworks (MOFs) have emerged as a promising class of materials due to their high surface area, tunable pore size, and versatile chemical functionality. This poster explores the synthesis, characterization, and application of functionalized MOFs in delivering therapeutic agents with enhanced efficacy and specificity. A two-step synthesis approach was employed to fabricate MOFs with tailored pore environments suitable for encapsulating hydrophobic and hydrophilic drugs. Advanced characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), and dynamic light scattering (DLS), were used to confirm the structural integrity and uniform size distribution of the MOFs. Functionalization with biocompatible ligands and surface coatings was achieved to improve stability in physiological conditions and enable targeted delivery. The poster also presents results from in vitro and in vivo studies demonstrating the controlled release of anticancer drugs, reduced cytotoxicity to healthy cells, and enhanced uptake by tumor tissues due to receptor-mediated endocytosis. The incorporation of imaging agents into MOFs for theranostic applications highlights their potential for simultaneous diagnosis and therapy. This research underscores the potential of nanostructured MOFs in advancing the field of precision medicine and suggests directions for future work in scaling up production and exploring synergistic therapies.

Abstract ID: ICCSHIP-2025/A-098

Formulation, Development and Evaluation of Antimicrobial Soap of Cnidoscolus Aconitifolius.

Mansi Bodharaj Lungase, Mayuresh Prakash Rajurkar
School of pharmacy, Swami Ramanand Teerth Marathwada University Nanded
*Email: - mansilungase2433@gmail.com, mayurpraj474@gmail.com

Abstract: The aim and objective of the present study are to formulate and evaluate anti-microbial herbal soap using Cnidoscolus aconitifolius. The antimicrobial activity of the prepared formulation was tested using agar well diffusion method against the organisms Staphylococcus aureus and they exhibited a good antimicrobial effect. The prepared formulation were evaluated for various physicochemical parameters for which good characteristics were observed. The easy availability of plants and their effectiveness helps manufacturers with cost effective benefits and with less or no side effects.

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Abstract ID: ICCSHIP-2025/A-099

A Study of Natural Dye and their Extractions

Rutuja Sanjay Sude, Sudarshani Bhagwan Patil
Dayanand Science College, Latur
*Email: - suderushikesh91@gmail.com

Abstract: Natural dyes are coloured compounds that are applied to a substrate such as fibre. Paper, cosmetics, hair etc to give colour and can be extracted from roots, fruits, bark, leaves, flowers, stem, fungi and lichens by various Processes of extraction. Natural dy es discuss thair sources. Properties and uses in textiles, food and Cosmetics. Most of natural dyes exhibit special Properties like anti-microbial, less toxicity, less allergic, Uv Protection and less side-effect and more effective. Natural dye Sources are ecofriendly and Permanent in fibrics. Prevent Pollution and other Harmfül effects. Demand of natural dyes has been incresed worldwide due to awareness about their beneficial properties.**Keywords:** Natural dye, eco-friendly, Textile

Abstract ID: ICCSHIP-2025/A-100

Green Nanoparticles as Emerging Tools in the Treatment of Breast Cancer: A Comprehensive Review

Shaikh Alfiya Gaffar, Sayed Nishat Munawar
Dayanand College of Pharmacy, Latur
*Email: - sayednishat2001@gmail.com

Abstract: Breast cancer remains one of the leading causes of cancer-related mortality in women worldwide, leading to the urgent need for innovative approaches to diagnosis and treatment. Green nanoparticles, synthesized through environmentally friendly methods using plant extracts or biological agents, have emerged as promising candidates in breast cancer therapy due to their unique properties that enhance their potential for biocompatibility, low toxicity, and multifunctional properties. This review explores the various types of green nanoparticles, including metallic (gold, silver, copper) and non-metallic nanoparticles (carbon-based, polymeric), highlighting their mechanisms of action in breast cancer treatment. The article also covers their potential as drug

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delivery systems, imaging agents, and hyperthermia treatment. Moreover, it examines the synergistic effects of green nanoparticles with conventional therapies such as chemotherapy, radiotherapy, and targeted therapies. The challenges of large-scale synthesis, stability, and regulatory approval are discussed, alongside future perspectives in clinical applications. Additionally, these nanoparticles can serve as efficient carriers for gene therapies or siRNA delivery to silence oncogenes associated with breast cancer progression. Despite their promising potential, challenges such as variability in synthesis, optimization of drug loading, and safety concerns remain. Overall, green nanoparticles present a promising, sustainable alternative in the fight against breast cancer, offering enhanced therapeutic efficacy and reduced side effects compared to traditional treatments. This review delves into the current state of nanoparticle research, its applications in breast cancer therapy and diagnosis, and the obstacles that must be overcome for clinical integration.
Key words: Green chemistry, Breast cancer, Nanoparticles, Metallic Nanoparticles.

Abstract ID: ICCSHIP-2025/A-101

Development and Evaluation of Gastro Resistance Multiple Units Pellets System Tablets

T. P. Tonge *, M. R. Gunde, J. R. Baheti
Department of Pharmaceutics, Rashtrasant Tukadoji Maharaj Nagpur University, Amravati Road, Gokulpeth, Nagpur -440033, MS, India
*Email: - tushartonge001@gmail.com

Abstract: The current study aims to develop and assess gastroresistant MUPS tablets. MUPS is believed to offer pharmacokinetic advantages than monolithic dosage formulations. The Wurster technique was used to create multiple unit dosage formulations. In order to create gastro-resistant MUPS tablets, first the sugar spheres (#18/20, #20/25, #30/35, and #40/60) were first coated with drug loading then barrier coating and enteric coating. Methacrylic acid copolymer solutions were use as enteric polymers. The dissolving rate, water content, acid resistance, and assay/drug concentration of the various pellet batches were assessed. The pellets were compressed directly into tablets with a binder, diluent, filler, disintegrant, and other suitable excipients. The study is to examine a number of physical attributes, including hardness, friability, diameter, thickness, disintegration time, dissolving test and assay, in order to evaluate and characterise the quality of tablets. Bigger sugar spheres will shatter against the coating more easily than smaller ones since they are less tolerant of the stomach environment. This leads us to the conclusion that little pellets were the most effective way to directly compress multiple unit particle systems.

Abstract ID: ICCSHIP-2025/A-102

Effect of Solvent and Amount of Catalyst on Synthesis of Benzimidazole Derivatives

Anil B. Chidrawar
P.G. Department and Research Centre of Chemistry,
Degloor College, Degloor. Dist: Nanded - 431717
*Email: - anilchidrawar74@gmail.com

Abstract: In the initial catalytic activity experiments, different solvents were screened for the reaction. Herein the reaction of benzaldehyde and orthophenylene diamine was selected as the

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model reaction. Solubility experiments showed that the cobalt (II) acetylacetone is miscible with methanol and relatively readily soluble in polar solvents such as ethanol, and they are partially immiscible with no-polar solvents such as ethyl acetate, and tetrahydrofuran. As shown in Table 1, the reactions could proceed effectively in polar organic solvents, such as methanol and ethanol (entries 1, 2), and cobalt (II) acetylacetone/CH3OH was found to be the most effective catalyst/solvent system and gave the highest yield of 97% (entry 1) among the solvents selected. The efficiency of the reaction was mainly affected by the amount of the catalyst. As can be seen from Table 2, the optimal amount of cobalt (II) acetylacetone was 0.05 mmol (entry 2). The isolated yield of 2-phenyl benzimidazole decreases with the increase of cobalt (II) acetylacetone from 0.05 mmol to 0.5 mmol

Key words: Cobalt (II) acetylacetone, methyl alcohol, 2-phenyl benzimidazole, ethyl acetate, tetrahydrofuran.

Abstract ID: ICCSHIP-2025/A-103

Simple and Efficient Synthesis of Fused Pyrimidine Derivatives and Study of their Biological Activity

Prashant N. Ubale[1], Sambhaji P. Vartale[2]
[1]Late Babasaheb Deshmukh Gorthekar Mahavidyalaya, Umri Dist. Nanded
[2]Yeshwant Mahavidyalaya Nanded Dist. Nanded, Maharashtra
*Email: - pupatil2015@gmail.com

Abstract: Pyrimidine is a nitrogenous base and one of the constituents of basic part of DNA. Apart from this pyrimidine with its derivatives shows various medicinal importance. Pyrimidines and its derivatives used as anticancer agent, antibacterial agent, antitumor activity, anticonvulsant and antithyroid activity. Such type of biological importance against different vital diseases, we prepared and studied the biological activity fused as well as different substituted pyrimidines.When substituted pyrimidines react with substituted methylene malononitrile in presence of K2CO3 and DMF then it gives substituted pyrimido pyrimidines. The formed pyrimido pyrimidines condensed with different active methylene compounds, heteryl amines, substituted phenols and amines to form corresponding derivatives of pyrimido pyrimidines. Then formed pyrimido pyrimidines evaluated for the study of antioxidant and antibacterial activity. Few of them shows the significant activity.

Abstract ID: ICCSHIP-2025/A-104

Kinematic Study of Viscosity Deviations of Binary Liquid Mixtures of Propionaldehyde with n-butanol Over All Compositions at 298.15, 308.15 and 318.15 K.

Satish B. Maulage
Vasantdada Patil Arts, Commerce & Science College, Patoda, Dist. Beed. (M.S.) India.
*Email: - satishmaulage@gmail.com

Abstract: Densities and viscosities of the binary mixtures of propionaldehyde with n-butanol at 298.15, 308.15 and 318.15 K over the entire range of all compositions have been measured using kinematic viscosity bath. From this experimental data, viscosity deviations ($\Delta\eta$), molar volumes V_m, excess molar volumes V^E and excess free energies of activation of viscous flow ΔG^{*E} have

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been determined. Viscosity deviations, excess molar volumes and excess free energies of activation of viscous flow were calculated and correlated Redlich-Kister polynomial equation.

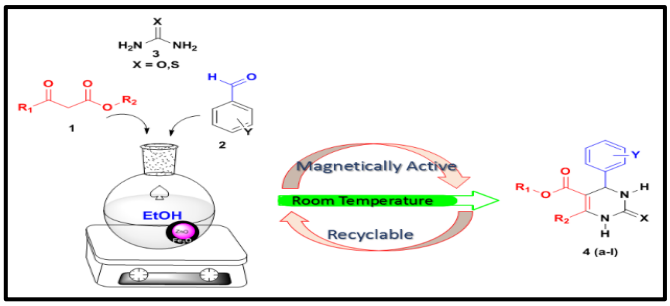
Key words: Density, Viscosity, Viscosity deviation, Excess molar volume, Binary system, propionaldehyde.

Abstract ID: ICCSHIP-2025/A-105

ZnO@Fe_3O_4-PNS: An Efficient, Magnetically Active and Recyclable Catalyst for Dihydropyirimidones Synthesis at Room Temperature

Sushil R. Mathapati
Department of Chemistry, Shri Madhavrao Patil Mahavidyalaya, Murum-413605
*Email: - sushilrswami@gmail.com

Abstract: Use of agriculture bio-waste in organic transformation is one of the greener and economical approach. Major population in India associated with agriculture sector, high amount of bio-waste have produced every year across the country and that cannot be reused or applied. Presently, we are working on utilization of such agriculture waste in the field of organic catalysis. With this dedication, herein we demonstrated the use of peanut shells bio-waste to form magnetically activated ZnO nano-composite as a heterogeneous, Lewis acid catalyst for dihydropyrimidones synthesis. Twelve derivatives were synthesized via one-pot cyclo-condensation of aromatic aldehydes, β-dicarbonyl and urea (thiourea) in attendance of ZnO@Fe3O4-PNS nano-composite at room temperature. ZnO@Fe3O4-PNS was introduced as an efficient magnetic nano-catalyst in Biginelli condensation with powerful reusability. The great (88-96%) yield of products, fast reaction time, simple work-up procedure, as well as usage of nontoxic, reusable, and easily recoverable catalyst with an external magnet was counted as advantages of the applied process. The magnetic nano-catalyst was removed after reaction completion and reused seven times at the same conditions without significant decay in catalyst activity. The magnetic nano-catalyst was synthesized through a simple and inexpensive two steps method and characterized by FT-IR, EDX, SEM, TEM, DLS, XRD, and VSM techniques. We believe that, present work will open innovative, efficient, economical and energy saving greener protocol for synthesis of dihydropyrimidones.



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Abstract ID: ICCSHIP-2025/A-106

Use of Cheminformatics Tools in Research and Developments

Ravindra S. Shinde,*[1] Vanita A. Navale*[2]
[1]Department of Chemistry, Dayanand Science College, Latur – 413 512, Maharashtra, India
[2]Department of Chemistry, VDF school polytechnic, College, Latur – 413 512, Maharashtra,
*Email: - vanitakadamnavale@gmail.com

Abstract: Research Scholars: Structure Drawing: ChemDraw, MarvinSketch, Database Search: PubChem, ChemSpider, Literature Search: SciFinder.Research Supervisors: Molecular Modeling: MOE, Gaussian, Schrodinger, Data Analysis: KNIME, OpenEye Research and Development: Crystal Structures: Cambridge Structural Database (CSD), Protein Structures: Protein Data Bank (PDB), Virtual Screening: AutoDock, ZINC, ChEMBL. The Cheminformatics toolkits are software development kits in computer applications for use in virtual screening, chemical database mining, and structure-activity relationship studies. There are many Cheminformatics toolkits which are useful for Research Scholar, Research Supervisor, Research and Developments which can be studied in this article.
Keywords: Cheminformatics, R and D, software development, Computational Chemistry.

Abstract ID: ICCSHIP-2025/A-107

Synthesis and Antimalarial Activities of New Hybrid Atokel Molecules

Kokane Balaji Digambar
Department of Chemistry Shri Kumarswami Mahavidyalaya, Ausa Dist.Latur,
*Email: bdkokane@gmail.com

Abstract: The currently spreading resistance of the malaria parasite Plasmodium falciparum to artemisinin-based combination therapies makes an urgent need for new efficient drugs. Aiming to kill artemisinin-resistant Plasmodium, a series of novel hybrid drugs named Atokels were synthesized and characterized. Atokels are based on an 8-amino- or 8-hydroxyquinoline entity covalently bound to a 1,4-naphthoquinone through a polyamine linker. These drugs have been designed to target the parasite mitochondrion by their naphthoquinone moiety reminiscent of the antimalarial drug atovaquone, and to trigger a damaging oxidative stress due to their ability to chelate metal ions in order to generate redox active complexes in situ.

Abstract ID: ICCSHIP-2025/A-108

Synthesis and Antimicrobial Activity of 2-(2-Arylamino-4-Phenylthiazol 5-yl)-5-Substituted Benzofuran Derivatives

Suryawanshi V. S. [1] Chavan J. L[2], Mugle Y.G[1]
[1]Dept. of Chemistry, P.G. and Research Centre, Shri Chhatrapati Shivaji College, Omerga
[2]API, R and D Centre, Emcure Pharmaceuticals Limited, Hinjewadi, Pune
*Email: vssurya11@gmail.com

Abstract: A series of 2-(2-arylamino-4-phenylthiazol-5-yl)-5-substituted benzofuran derivatives were synthesized from 1-aryl-3-(N-phenylbenzimidoyl)thiourea and 2-(2-bromoacetyl)-5-substituted benzofuran in the presence of triethylamine. Their structure was established on the basis of IR,1H NMR and Mass spectral techniques. The entire newly synthesized compounds

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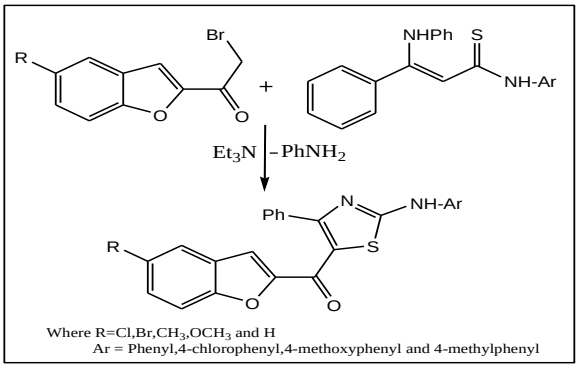
were screened for their antifungal and antibacterial potential. All the compounds showed low to moderate activity against the microorganisms tested.

Reaction Scheme:



Abstract ID: ICCSHIP-2025/A-109

Genomic Medicine

Barkul Prachi Sunil, Agashe Aditee Rushikesh
Dayanand College of Pharmacy, Latur.
*Email: - adibande007@gmail.com

Abstract: Genomic medicine is rapidly changing the future of medicine. Medical librarians need to understand this field of research and keep current with its latest advancements. Even if they are not directly involved in genomic medicine, librarians can play an integral role by helping health care consumers and practitioners who may also need to expand their knowledge in this area. This article provides a basic introduction to genomic medicine, gives a brief overview of its recent advancements, and briefly describes some of the ethical, legal, and social implications of this emerging area of research and practice.

Keywords: Genomic medicine, Advancement, Emerging science, Practice

Abstract ID: ICCSHIP-2025/A-110

Green Synthesis of Functionalized 2, 3,7,8-Tetrahydro-4H, 6H Pyrano[3,2-g] Chromene-4,6-Diones Using TSIL[SBMIM]Cl

Barkul Prachi, Motegaonkar Manorama
Department of Chemistry Azad Mahavidyalaya, Ausa.
*Email: - manoramamotegaonkar42@gmail.com

Abstract: A fast, highly efficient and green protocol for the synthesis of functionalized 2,3,7,8-tetrahydro-4H,6H-pyrano [3,2-g]chromene-4,6-dionesat room temperature has been investigated using task-specific acidic ionic liquid (TSIL), 1-(4- sulfobutyl)-3-methyl imidazolium chloride [SBMIM]Cl-, as catalyst and green reaction medium. The reactions precede with excellent yields in short reaction times. The TSIL can be recycled for subsequent reactions with consistent activity.

Keywords: chalcones, flavanones, Kabbe condensation, Task specific basic ionic liquid

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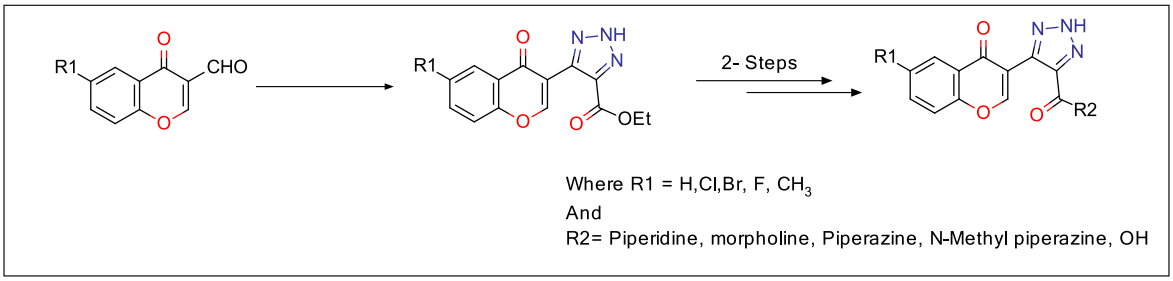
Abstract ID: ICCSHIP-2025/A-111

Synthesis, and Biological Evaluation of Triazole Linked Chromone Derivatives.

Gurpinder Singh*, Raj Kumar
1Department of Chemistry, Lovely Professional University, Punjab-144411.
*Email: - gurpinder.singh@lpu.co.in

Abstract: Triazole linked chromone-cyclic amines hybrids containing three heterocyclic rings were synthesized from affordable starting materials such as substituted 3-formylchromones. Substituted 3-formylchromones were converted to triazole derivatives with simple metal free techniques and isolated in good yields. These derivatives were further subjected to modification through multistep synthesis to include another heterocyclic ring via amide bond to obtain new hybrids which includes chromones as core ring, triazole as linking change and cyclic amine as side chain. All the molecules were characterized by spectroscopic techniques such as NMR, IR and mass. These molecules have been evaluated for antimicrobial and antifungal activities. Some of the molecules have shown good to excellent activities.

Keyword: Triazole, Chromone, Triazole, Amide linkage, Antimicrobial



Abstract ID: ICCSHIP-2025/A-112

Bio-priming: A Revolutionary Thought Against Chemicals-Based Crop Improvement.

Yadav S.G.
Department of Botany, Shivaji Mahavidyalaya Renapur Dist. Latur:- 413527 M. S. INDIA
*Email: dryadavsg@gmail.com

Abstract: The ideal methodology that can be used for rendering resistance to plants against various stressful situations is priming. Exposure of crops to stress is the most significant barrier to agricultural output and food security worldwide. Stress induces changes in plants physiological functions, which leads to lower plant growth and agricultural yield. In priming, physiological state of seeds can be changed by treating with various priming agents like water, chemical and biological organisms. Various microorganisms including plant growth promoting bacteria and fungi are successfully used for bio-priming in plants. Because of the eco-friendly nature of bio-priming, it becomes an apt method that can be practiced for the future for stress alleviation in crops. It imparts both abiotic and biotic stress tolerance in plants. Agriculture sector has been dramatically depending on the chemical pesticides and fungicides for eradicating pathogenic attacks. Bio-priming is a

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promising strategy for imparting various biotic/abiotic stresses thus paving way for the removal of chemicals from crop protection.

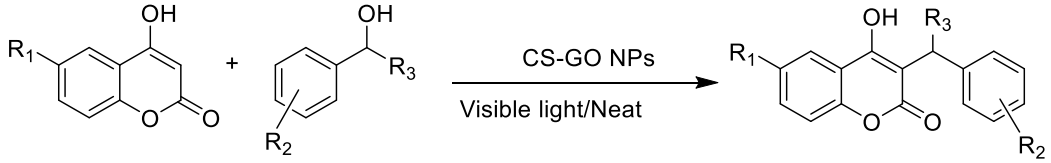
Key-Words: Bio-priming, Plant growth promoting microbes, Agriculture, Stress.

Abstract ID: ICCSHIP-2025/A-113

C-alkylation of 4-Hydroxycoumarin with Activated Alcohols Using CS-GO Nanoparticles as a Photo-catalyst Under Visible Light Irradiation

Girdharilal Tiwari[1], Tabassum Siddiqui[2], Zubaidha Pudukulathan[2]*
[1]Department of Chemistry, J. M. Patel Arts, Commerce & Science College, Bhandara - 441904, Maharashtra, India
[2]School of Chemical Sciences, Swami Ramanand Teerth Marathwada University, Nanded– 431606, Maharashtra, India
*Email: girdharilal77@gmail.com

Abstract:A visible-light promoted, highly efficient and selective procedure was developed for the synthesis of a C-3 alkylated derivative of 4-hydroxycoumarin under mild reaction conditions using various functionalized primary and secondary alcohols in the presence of catalytic amount of carbonised sugar graphene oxide (CS-GO) nanoparticles.



R3=alkyl,aryl,alkenyl,alkynyl

Keywords: Carbonized sugar, visible light, 4-hydroxycoumarin, c-alkylation.

Abstract ID: ICCSHIP-2025/A-114

Preparation and Characterization of g-C3N4/MCM-41 Composite Catalysts for Photocatalytic Applications

N. B. Kale, A. L. Ghodke, Dr V. S. Suryawanshi*, Dr M. K. Patil*
Department of Chemistry, Dr Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Sub-Campus Dharashiv-413501, MS, India
Chhatrapati Shivaji College, Omerga-4135606, MS, India
*Email: - meghshyam_patil@yahoo.com

Abstract: A metal-free polymeric photocatalyst has been considered as a promising material for solar energy utilization because of its desirable band gap. In this work, we have synthesized gC3N4/MCM-41 composite photocatalysts by using sol-gel method. Three different gC3N4/MCM-41 composite photocatalysts by varying the percentage of g-C3N4 i.e. 5%-gC3N4/MCM-41, 10%-g-C3N4/MCM-41, and 20%-g-C3N4/MCM-41. Prepared series of catalysts have been characterized by XRD and FT-IR spectroscopy. These catalysts can be applied for photocatalytic degradation organic pollutants.

Keywords: Composites, g-C3N4/MCM-41, Photocatalytic Degradation

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Abstract ID: ICCSHIP-2025/A-115

Phytomedicines Are Used In The Treatment of Malaria

Taher Farid Shaikh[1], Kiran Ashok Hanwate[2]
Nanded Pharmacy College, Nanded, Maharashtra, India
*Email: shaikhtaher5000@gmail.com

Abstract: Malaria causes approximately one million deaths annually, posing significant challenges in its treatment. Despite extensive research, the development of a viable vaccine remains elusive due to the complex metabolic pathways in the parasite's life cycle. However, nature offers an untapped reservoir of secondary metabolites that hold promise for antimalarial drug discovery. Traditionally, plant-based medicines have been utilised to treat malaria, suggesting that plantderived compounds could be potential lead molecules for developing novel antimalarial drugs. This study highlights six plant species Alstonia scholaris, Coptis teeta, Crotolaria occulta, Ocimum sanctum, Polygala persicarioefolia, and Vitex peduncularia commonly used in different regions of India.
The most frequently utilised plant parts include leaves (33%), roots (31%), bark, and the whole plant (12%). These findings provide a foundation for further research to identify and develop effective antimalarial agents from these plant species.
Keywords: Malaria, Medicinal Plants, Mosquito Repellent, Alkaloids, Traditional Knowledge of Medicines, Plasmodium Falciparum.

Abstract ID: ICCSHIP-2025/A-116

A Study on Advances in Organic Synthesis and Methodology

Kote A. M[1]., Tekale A. S.[2], Reddy P. S. [2] Muley D. B.[2]
[1]Chemistry Department, PG students in Shivaji Mahavidyalaya, Udgir.
[2]Faculty in Chemistry Department Shivaji Mahavidyalaya, Udgir.
Department of Chemistry & research centre, Shivaji Mahavidyalaya, Udgir.
*Email: - aishwaryakote7@gmail.com

Abstract: Organic synthesis continues to drive a broad range of research advances in chemistry and related sciences. Another clear trend in organic synthesis research is the increasing desire to target improvements in the quality of life of humankind, new materials, and product specificity. Here, a landscape view of organic synthesis research is provided by analysis of the CAS Content Collection. Three emerging research directions, enzyme catalysis, photocatalysis, and green chemistry in organic synthesis, were identified and featured based on the publication trend analysis. The realm of organic synthesis continues to witness remarkable advancements, driven by the quest for more efficient, sustainable, and versatile methodologies. This paper delves into recent breakthroughs and emerging trends in organic synthesis methods. Emphasizing the importance of sustainability and selectivity, researchers have developed novel strategies that encompass diverse transformations, catalytic systems, and reaction mechanisms. From transition-metal-catalyzed cross-coupling reactions to organocatalysis and biocatalysis, the landscape of organic synthesis has expanded significantly, offering new avenues for the construction of complex molecular architectures with high precision and atom economy. Furthermore, the integration of computational

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tools and automation has revolutionized reaction optimization and design, enabling rapid exploration of chemical space and accelerating the discovery of innovative synthetic routes. This paper provides an overview of key developments, challenges, and future prospects in the field of organic synthesis, highlighting the pivotal role of interdisciplinary approaches and collaborative efforts in driving scientific progress and addressing societal needs.

Keywords: Organic synthesis, advances, methodologies, sustainability, catalysis, selectivity, automation, computational tools, innovation, Green Chemistry.

Abstract ID: ICCSHIP-2025/A-117

Formulation & Evaluation of Herbal Sunscreen Lotion

S. A. Nagrale*, S. S. Borkar, J. R. Baheti

Department of Pharmaceutics, Rashtrasant Tukadoji Maharaj Nagpur University, Amravati Road, Gokulpeth, Nagpur -440033, MS, India

*Email: - nagrales27@gmail.com

Abstract: Sunscreen lotion is a sort of product that protects against the sun's harmful rays by containing ultraviolet radiation (UV rays), which is divided into two types: ultraviolet radiation A (UVA) and ultraviolet radiation B (UVB). The incorporation of herbal materials into sunscreen is one of the most effective and natural ways to protect against the sun, as measured by the sun protection factor (SPF), as well as the detrimental side effects of toxic chemicals. The present study aimed to develop herbal sunscreens containing turmeric (strong antiseptic property which protects skin from bacteria caused by excess sweat), coconut oil (used as a sun-block agent and helps to protect skin from sun damage), aloe vera (give a cooling effect to the skin and work as skin barrier), lemon (used to protect skin for sunburn) which will be effective for skin and protect skin against harmful sun rays, sunburn, and skin cancer. Prepared herbal sunscreens were evaluated for physicochemical characteristics, SPF, Viscosity, Extrudability, pH, anti-microbial activity, and stability. Results showed that the F4 and F2 herbal sunscreens were of good consistency and viscosity with excellent antioxidant, non-mutagenic, non-irritant, stability activity and possessed 33.50 SPF for normal skin. In comparison to F1 through F3, formulations with a coconut oil base and (F4 and F2) were shown to be stable and effective, with a high SPF.

Abstract ID: ICCSHIP-2025/A-118

Multicomponent Synthesis of Substituted Derivatives of 1, 3, 4 Thiadiazole

Kotalwar S.S.[1], Kale A. D.[1], Jagrut V. B.[2]

[1] Department of Chemistry, Lal Bahadur Shastri Senior College Partur, Jalna, Maharashtra, 431501 India

[2] Department of Chemistry, Swami Vivekanand Sr. College, Mantha, Jalna, Maharashtra, 431501 India

*Email: - nagrales27@gmail.com

Abstract: It deals with the multicomponent synthesis of substituted derivatives of Multicomponent synthesis of 2-substituted derivatives of 1, 3, 4-thiadiazole. A mixture of 1, 3, 4-thiadiazole (1) and

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ethyl-2-cyano-3, 3-bis (methylthio) acrylate (2) was refluxed in dimethyl formamide and anhydrous potassium carbonate to isolate derivatives of 1, 3, 4-thiadiazole. The formed compound was reacted with different aryl amines/phenols/heteryl amines and compounds containing active methylene group independently to form different substituted derivatives of 1, 3, 4-thiadiazole. Structures to these newly synthesized compounds were assigned on the basis of elemental analysis and spectral data.
Keywords: 1, 3, 4-thiadiazole, Heteryl amines, potassium carbonate.

Abstract ID: ICCSHIP-2025/A-119

Microwave Assisted Simple & Rapid Synthesis of Pyrazol Pyran Derivatives & Their Biological Study

M. P. Munde[1], S. N. Niwadange[2], S. S. Mahurkar[1]
[1]Department of Chemistry, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA
[2]Dept. Of Chemistry, Shri Govindrao Munghate Arts and Science College, Kurkheda, Maharashtra,
*Email: - shreyas.mahurkar@gmail.com

Abstract:A rapid and environmentally friendly procedure has been developed for the preparation of pyrazole-pyran derivatives using a phase transfer catalyst in aqueous medium. The target compounds were synthesized through reaction of 1-phenyl, 3-methyl-5-pyrazolone with aromatic aldehydes under microwave irradiation. The synthesized compounds were characterized by NMR, IR, and mass spectra, to confirm their structure and purity. This method offers several advantages such as short reaction time, high efficiency, an inexpensive and easy-to-handle catalyst, avoidance of organic solvents, and simple work-up that they are consistent with green chemistry.
Keywords: Microwave, aldehyde, pyrazol pyran derivatives, PTC, biological activity.

Abstract ID: ICCSHIP-2025/A-120

Green Chemistry: A Review

Mane A. B., Tekale A.S, Reddy P.S., Muley D. B.
Chemistry Department, PG students in Shivaji Mahavidyalya Udgir, (MH)-413517
*Email: akankshamane13928@gmail.com

Abstract: Chemical goods and processes that are created from the ground up by principles that make them favorable to life will serve as the material foundation upon which a sustainable society will be built. To determine whether compounds and processes are depleting or renewable, harmful or benign, and persistent or rapidly degradable, it is necessary to take into consideration the important intrinsic features of molecules from the very beginning, which is the design stage. The ideas of green chemistry and green engineering will need to be incorporated into products, feedstocks, and manufacturing processes to meet the requirements of an enlarged definition of performance that considers sustainability considerations. To accomplish this change, it will be necessary to combine the most successful aspects of scientific and innovative traditions with the most recent developments in systems thinking and design. This transformation will begin at the molecular level and will ultimately have a positive impact on a global scale.
Keywords: Food technology, Green Chemistry's Principles, Pharmaceuticals, Sustainable Chemistry

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Abstract ID: ICCSHIP-2025/A-121

Review on Design of Experiment Applied to Pharmaceutical & Analytical Quality by Design

Mayuri Patil, Aarti Khandekar, Rachana Maniyar
Dayanand College of pharmacy, Latur
*Email: rachanamaniyar4@gmail.com

Abstract: Designs of Experiments (DoE) play a pivotal role in Pharmaceutical and Analytical Quality by Design (AQbD), ensuring the development of high-quality, robust products and processes. In the pharmaceutical industry, DoE methodologies are used to systematically evaluate the impact of multiple variables on product quality and performance, thereby identifying critical quality attributes (CQAs) and optimizing manufacturing processes. AQbD integrates these principles into the analytical development phase, where DoE is applied to improve the precision, accuracy, and sensitivity of analytical methods. This paper explores the application of DoE in pharmaceutical and analytical development, highlighting its role in identifying and controlling variability, optimizing experimental conditions, and ensuring product consistency. Case studies are presented to demonstrate the benefits of DoE in process optimization, method validation, and risk assessment, underscoring its importance in the implementation of the pharmaceutical quality system. The integration of DoE with AQbD offers a structured approach to developing products that meet regulatory standards and deliver consistent therapeutic performance, ultimately advancing the goal of ensuring patient safety and efficacy.

Abstract ID: ICCSHIP-2025/A-122

Metrics for Green Chemistry in the 21st Century

K. I. Mominn,[1] V. S. More[2], G. R. Nagargoje[3], P. D. Kadam[4], A. S. Bondge[5*]
[1]Dept. of Chemistry, Rajarshi Shahu Mahavidyalaya, Latur, Dist-Latur, 413512
[2]Dept. of Chemistry, Kai. Rasika Mahavidyalaya, Deoni, Dist-Latur, 413519
[3]Dept. of Chemistry, Shivaji Mahavidyalaya, Renapur, Dist-Latur, 413527
[4]Dept. of Chemistry, Shri Kumarswami Mahavidyalaya, Ausa Dist Latur, 413520
[5]*Dept. of Chemistry, Shivneri Mahavidyalaya, Shirur Anantpal Dist Latur, 413544
*Email: abhaybondge@gmail.com

Abstract: Green chemistry has emerged as a transformative approach to designing chemical processes and products that prioritize sustainability and minimize environmental impact. As the 21st century presents pressing challenges such as climate change, resource depletion, and pollution, robust metrics are crucial for evaluating the implementation and success of green chemistry principles. This paper explores key metrics, including atom economy, the E-factor, lifecycle analysis, renewable resource utilization, and energy efficiency, which serve as quantitative tools to measure the environmental and economic performance of chemical processes. Advances in computational tools, artificial intelligence, and big data analytics are enhancing the accuracy and applicability of these metrics, driving innovation in industrial practices. The research also examines the role of metrics in shaping policy, encouraging industry adoption, and aligning with global sustainability goals. By standardizing and integrating these metrics into decision-making

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frameworks, green chemistry can accelerate its impact in addressing the environmental challenges of the 21st century. We discuss the evolution of these metrics, their application in various industries, and their role in fostering innovation while minimizing environmental impact. Through this exploration, we aim to underscore the importance of standardized, comprehensive metrics for advancing Green Chemistry.

Keywords:- Green Chemistry, sustainability metrics, environmental impact, 12 principles of Green Chemistry, life cycle assessment, atom economy, E-factor.

Abstract ID: ICCSHIP-2025/A-123

Sugar and Alcohols: Mannitol, Sorbitol, Xylitol, and Erythritol

Biradar Mohan Bhimrao[1], Panchal Bapurao Dagdu[1], Tekale A.S.[1], Reddy P.S.[2]
[1] Chemistry Department, PG students in Shivaji Mahavidyalaya, Udgir
[2]Faculty in Chemistry Department Shivaji Mahavidyalaya, Udgir
*Email: biradarmohan548@gmail.com

Abstract: The sugar alcohols commonly found in foods are sorbitol, mannitol, xylitol, erythritol, isomalt, and hydrogenated starch hydrolysates. Sugar alcohols come from plant products such as fruits and berries. Sugar alcohols occur naturally and at one time, mannitol was obtained from natural sources. Today, they are often obtained by hydrogenation of sugars and other techniques. Sugar alcohols do not contribute to tooth decay. Consumption of sugar alcohols may affect blood sugar levels, although less than of sucrose. Mannitol and sorbitol are isomers, the only difference being the orientation of the hydroxyl group on carbon among production methods of mannitol are Industrial synthesis, Biosyntheses, Natural extraction, chemical process, microbial process. Most sorbitol is made from corn syrup, but it is also found in apples, pears, peaches, and prunes. It is converted to fructose by sorbitol-6-phosphate 2-dehydrogenase. Xylitol is a "tooth-friendly", nonfermentable sugar alcohol. It appears to have more dental health benefits than other polyalcohols. The structure of xylitol contains a tridentate ligand, $(H\text{-}C\text{-}OH)_3$ that can rearrange with polyvalent cations like Ca^{2+}. This interaction allows Ca^{2+} to be transported through the gut wall barrier and through. Xylitol is produced by hydrogenation of xylose, which converts the sugar (an aldehyde) into a primary alcohol. Another method of producing xylitol is through microbial processes, including fermentative and biocatalytic processes in bacteria, fungi, and yeast cells, which take advantage of the xylose-intermediate fermentations to produce high yield of xylitol. In the body, most erythritol is absorbed into the bloodstream in the small intestine, and then for the most part excreted unchanged in the urine. About 10% enters the colon. Because 90% of erythritol is absorbed before it enters the large intestine, it does not normally cause laxative effects. Chemical and fermentative processes have been introduced for large-scale production of erythritol. Erythritol can be synthesized from dialdehyde starch by high-temperature chemical reaction in the presence of a nickel catalyst.

Keywords: xylitol, Erythritol, biofuels, sorbitol, mannitol, biorefinery, thermal integration,co-products, sustainable development

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Green HPLC Methods for the Identification of Pharmaceutical Products: Development, Validation and Green Evaluation

Nikita P. Sirsikar[1], Anuja V. Chate[2], R. S. Sakhare [1,2],*

[1] Department of Quality assurance, Channabasweshwar Pharmacy College (Degree), Latur,

[2]Department of Quality Assurance, Channabasweshwar Pharmacy College (Degree),

Latur – 413 512, Maharashtra.

*Email: nikitashirsikar@gmail.com

Abstract: Today's conditions that directly affect the environment, it is vital to develop more environmentally friendly analytical methodologies. Therefore, the use of environmentally friendly chemicals is becoming more popular in all analytical techniques, including liquid chromatographic methods. Developing environmentally friendly methods to prevent environmental pollution, reducing energy consumption and waste management has become even more critical for the future of humanity in a world where clean water resources are rapidly decreasing and air pollution is a significant problem, the effects of global warming and climate change are more evident. It is thought that the method developed with this thought can be considered an environmentally friendly alternative to the methods currently used in the quantification in pharmaceutical products in the pharmaceutical industry. The proposed method can be considered an advantageous and innovative method in the application of green analytical chemistry, being an alternative ecologically safe and correct to be used in routine quality control analysis. This method will be very useful in future perspective.

Abstract ID: ICCSHIP-2025/A-125

Development and Evaluation of Alginate Microspheres by Using Model Drug

Ssbe's Nanded Pharmacy College, Nanded.

Bembalge Nikita Baburao, Kalbande Snehal Parmanand

*Email: nikitashirsikar@gmail.com

Abstract: The development of controlled-release formulations has been significantly enhanced by the use of microspheres, which offer a promising alternative to conventional drug delivery systems. This study investigates the effect of various types and concentrations of cross-linking agents on alginate microspheres, which were prepared using the ionic gelation technique. Paracetamol was used as a model drug. The microspheres were evaluated for several parameters, including drug content, bulk density, tap density, and Carr's index. Microspheres, with diameters ranging from 1 to 1000 µm, are considered novel drug delivery systems that provide effective therapeutic alternatives to immediate-release dosage forms. The study highlights the impact of different preparation techniques on the effectiveness and administration of the dosage forms. Microspheres were characterized through various evaluation methods to assess their quality. The findings suggest that alginate microspheres hold significant potential as a central component in the future of novel drug delivery systems.

Keywords: Paracetamol, Microspheres, Sodium alginate, Calcium.

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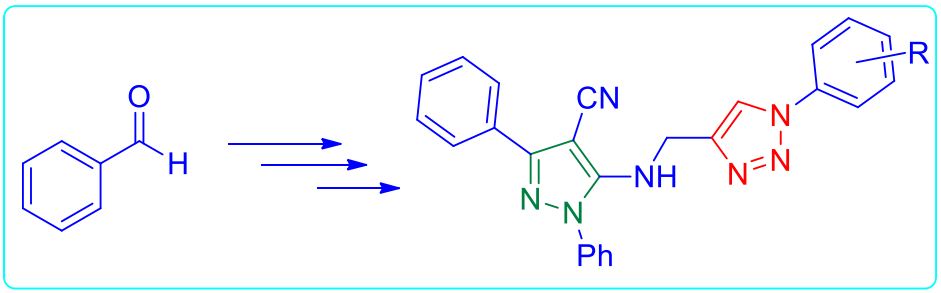
Abstract ID: ICCSHIP-2025/A-126

Efficient and Green Synthesis of Pyrazole-Triazole Derivatives

Nitin B. Haval, Giribala M. Bondle*
Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar
*Email: gmbondle@gmail.com

Abstract: Pyrazoles are privileged heterocyclic moieties in various natural products, pharmaceutical compounds, agrochemicals, functional organic materials. This work describes DABCO catalyzed efficient and green synthesis of new pyrazole-triazole derivatives. All the newly synthesized compounds were characterized by using various spectral techniques like IR, 1H NMR, 13C NMR and Mass spectra. The main advantage of this synthesis is clean reaction, high efficiency, use of less toxic catalyst, low cost and environment friendly solvents.



Keywords: DABCO, Pyrazole, Triazole, Knoevenagel condensation.

Abstract ID: ICCSHIP-2025/A-127

Investigating the Anti-Cervical Cancer Potential of Cardiospermum Halicacabum Leaf Extract: An Integrated In-vitro and In-silico study with OHRLCMS Based Phytochemical Analysis

Padmaja Onkar*, Rajashri Khamkar*, Shamal Jaiswal, Dr. R. B Gholve
School of Pharmacy S.R.T.M.U., Nanded
*Email: padmajaonkar@gmail.com

Abstract: Cancer is the second leading cause of death worldwide, killing approximately 3500 per million people each year. This study aimed to explore the anti-cervical cancer potential of Cardiospermum halicacabum through an in vitro study on the HeLa CCL2 cell line. Additionally, it sought to construct possible compound/target/pathway biological networks for anti-cervical cancer effects using a docking-weighted network pharmacological approach and to investigate its potential mechanism of action. Ultra-sonication extraction of Cardiospermum halicacabum leaves was performed, identifying 1294 natural compounds via O-HRLCMS, with 294 compounds screened. Cervical cancer-associated gene targets were retrieved from databases, and their functions with related pathways were examined. Networks were built using Cytoscape v3.7.2, and ligand docking was performed with Autodock tools. Swiss ADME and Pre ADMET analysed pharmacokinetic properties. An in vitro study confirmed the anti-cervical cancer activity. Our findings indicate that

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the anticancer activity of Cardiospermum halicacabum involves 9 compounds and 10 targets, forming significant networks. Molecular docking estimated the binding affinity of protein-ligand complexes, with 19- Nortestosterone showing highest binding affinity (-8.4) than standard with 5F19. The In-vitro study using the HeLa CCL2 cell line demonstrated significant anticancer activity of the extract.
Key Words: Cervical cancer, Cardiospermum halicabum, HeLa CCL2

Abstract ID: ICCSHIP-2025/A-128

Formulation and Evaluation of Herbal Shampoo for Scalp Health & Hair

Surayya J. Patel, Anam A. M. Sigapure, A. B. Mane*,
Research Centre in Chemistry, Department of Chemistry, Dayanand Science College,
Latur-413512, Maharashtra, India.
*Email: surayyapatel551@gmail.com

Abstract: This study focuses on the formulation of a herbal shampoo using natural plant-based ingredients such as AloeVera, Neem, Hibiscus, Amla, known for their benefits to scalp health and hair care. The shampoo was developed to provide a gentle yet effective cleansing experience, promoting healthy hair growth and reducing scalp issues like dandruff and dryness. The formulated herbal shampoo offers a natural, eco-friendly alternative to traditional synthetic shampoo, providing nourishment and enhancing hair quality without harmful chemicals.

Key Words: Herbal Shampoo, Scalp Health and Hair, Organic and Plant-based ingredients.

Abstract ID: ICCSHIP-2025/A-129

Chemistry of Perfumes (Synthetic & Natural)

Yogeshvari R Lamture, Ravindra S. Shinde*,
Department of Chemistry, Dayanand Science College, Latur-413512, Maharashtra, India
*Email: rshinde.33381@gmail.com

Abstract: Perfumes have been an integral part of human culture for centuries, with a vast array of fragrances available in the market. However, the science behind perfume creation remains a mystery to many. This abstract delves into the chemistry of perfumes, exploring the fundamental principles and chemical compounds that contribute to the intricate world of fragrances. The

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synthesis and formulation of perfumes involve the combination of natural and synthetic ingredients to create unique fragrances. This study explores the synthesis and formulations of synthetic and natural perfumes. Synthetic perfumes are formulated using aroma compounds, such as aldehydes, esters, and terpenes, which are synthesized through various chemical reactions.

Key Words: Perfume synthesis, Fragrance chemistry, Natural perfumes, Synthetic perfumes, Aroma compounds, Essential oils

Abstract ID: ICCSHIP-2025/A-130

Formulation and Evalution of Harbal Kajal: A Natural Alternative

Adsul Nisha, Anuradha shinde
Department of Biotechnology, Dayanand Science College, Latur-413512, Maharashtra, India
*Email: pratikadsul85@gmail.com

Abstract: Kohl is a revolutionary technique and a novel are conceived of as the production of Kohl herbal kajal. Kajal is the most popular items. In India, kohl has been used for cosmetic purposes for centuries it is use as cosmetic and treats the eye problems. Kajal, also referred to as Surma or kohl, is used as an eye-catching accessory. The aim of the preparing formulation that is medicated herbal kajal is to treat eye inflammation and eliminate redness of the eye. Stability and patient-friendly nature are the main advantages of these products. The key benefits of these Cosmetics items are greater patient conformity, water-resistant properties, durability and cost-efficient shaping Curve. The medicinal products Triphala, Rose water, Almonds powder, Coconut oil, dill seeds, camphor and Ghee are used to formulate the herbal kajal. Utilizing two therapeutic ingredients and viz. dill seed and camphor set out to determine each other's ability to administer herbal kajal for an extended period of time Kohl's have been used since antiquity in various civilizations of the world, and dates back to the Bronze Age. It is chiefly used by the females of South Asia, Middle Eastand Africa. It is known as "qwalli" in West Africa and "Surma", "kajal", or "kaadige" in South Asia. The concerns are even more grave since kohl finds greater acceptability in women and infant population. Herbal kohl was formulated and scientific intent was used for selection of ingredients. Evaluation of the medicated herbal kajal is carried out by using the different parameter like pH, Spreadability, Physical evaluation etc. The formulation of kajal using various oils and additives, and multiple evaluation tests. Physical evaluation of the kajal includes assessments of color, odor, texture, and consistency, all of which met the desired criteria. The pH determination showed an average pH of 7.18, indicating suitability for skin application. Skin irritation tests confirmed the kajal's safety, with no irritation observed. Spreadability tests revealed optimal spreadability, ensuring smooth application. Stability studies showed no changes in the product's characteristics at room temperature and 40°C, indicating good shelf-life. The evaluation of the base, specifically cow ghee, included acid, saponification, and ester values, confirming its quality. Prepared medicated herbal kajal are evaluated by antimicrobial activity.

Key Words: kajal, Triphala, Rose water, Almonds powder

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Abstract ID: ICCSHIP-2025/A-131

Formulation and Evaluation of Bioplastic Strips Using Different Starch

Pratik Lomate[1], Sarita Mohite[2]

[1] Department of Pharmaceutical Quality Assurance, Channabasweshwar Pharmacy College (Degree), Latur – 413 512, Maharashtra, INDIA

[2]Department of Chemistry, Channabasweshwar Pharmacy College (Degree), Latur – 413 512, Maharashtra, INDIA

*Email: lomatepratik1@email.com

Abstract: Due to the negative environmental impacts of synthetic plastics, the development of biodegradable plastics for both industrial and commercial applications is essential today. The present work investigates the starch-based bio plastics for packaging applications various samples of bio plastics are produced, with different compositions of starch, glycerol, citric acid, and gelatin. However, water absorption and water solubility were reduced. Apart from Starch we can also use chitosan, cellulose and protein extracted from renewable biomass, but in our research proposal we will restrict our discussion to combination of starch, to which we can add other supplementary ingredients which would further improve the properties of the finished product in terms of its comfort during use and, it is physical appearance. Our prime goal here is to basically come up with a product that causes least damage to the surroundings. On the basis of these results, the best sample was analyzed for thickness testing, biodegradability properties, water solubility, moisture content and swelling properties of bio plastic.

Abstract ID: ICCSHIP-2025/A-132

Green Beauty: A Formulation of Natural lipstick

Pratiksha Supekar, Nitin Chauhan

Department of Biotechnology, Dayanand science college, Latur MS. (India)

*Email: pratikshasupekar5@gmail.com

Abstract: The cosmetic industry has been growing trend toward natural and eco-friendly products, with lipsticks being one of the most popular items. Natural lipstick are made using ingredients derived from plant, minerals and other organic sources, offering a safer alternative to Chemical-laden products. The primary components include natural oils like coconut, almond, which provide moisturization and smooth texture. Natural waxes such as beeswax or candelilla wax are used to give structure and firmness to the product. For pigmentation, natural colorants like beetroot powder, cocoa, and turmeric are commonly utilized. Essential oils like peppermint or lavender add a pleasant fragrance and offer therapeutic benefits. These lipstick are free from synthetic dyes, parabens, and heavy metals, making them suitable for sensitive skin. The process involves melting and blending the waxes and oils, followed by the addition of pigments and fragrance. This formulation not only provides hydration and vibrant color but also contributes to sustainability and environmental responsibility, promoting healthier cosmetics choice.

Keywords: Beeswax, Beetroot juice, Glycrine

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Abstract ID: ICCSHIP-2025/A-133

Exploration of Structural, Optical, Magnetic Characteristics of Nickel Doped Lithium-Yttrium oxide Nanoparticles

R.B. Bhore[1], M.M.Gurav[1], P.B. Jagtap[1], S.G. Mudbikar[1], P.D. Chaudhari[1], S.C.Waghmare[1], R.B. Bhakte[1], Y.P. Sarnikar[2], R.M.Tigote[1]*

[1]Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Sub Campus Dharashiv, Maharashtra-413501, India

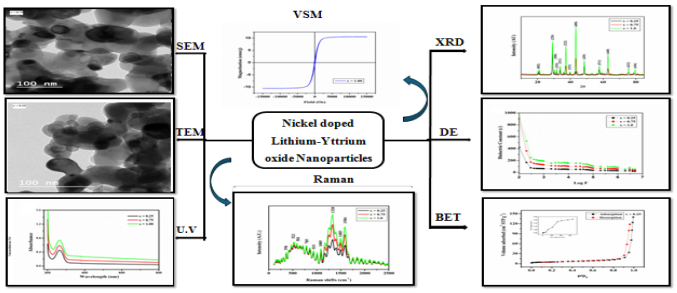
[2]Department of Chemistry, Dayanand Science College, Latur - Maharashtra-413512, India

*Email: rmtigote.chemobad@bamu.ac.in

Abstract: The sol-gel auto-combustion method successfully synthesized nickel-doped lithium-yttrium oxide nanoparticles. The synthesized samples structural study was annealed at 600°C for 6 hours and are characterized by ultraviolet spectroscopy (UV) results, the optical band gap between 2.50 eV and 2.38 eV. In the X-ray diffraction (XRD) analysis, it was revealed that the lattice parameter decreased from 8.3952 to 8.3329 Å with an increase in the doping weight percentage of Ni^{2+} ions. The morphology with elemental composition was investigated by SEM-EDS analysis and the electromagnetic properties were studied.

Keywords: Magnetism, Nanoparticles, Optical properties

Graphical abstract



Abstract ID: ICCSHIP-2025/A-134

Investigating the Anti-Cervical Cancer Potential of Cardiospermum Halicacabum Leaf Extract: An Integrated In-Vitro and In-Silico Study with OHRLCMS Based Phytochemical Analysis

Rajashri Khamkar*, Padmaja Onkar*, Shamal Jaiswal, R. B Gholve

School of Pharmacy SRTMU, Nanded

*Email: rajshri99kk@gmail.com

Abstract: Cancer is the second leading cause of death worldwide, killing approximately 3500 per million people each year. This study aimed to explore the anti-cervical cancer potential of Cardiospermum halicacabum through an in vitro study on the HeLa CCL2 cell line. Additionally, it sought to construct possible compound/target/pathway biological networks for anti-cervical cancer effects using a docking-weighted network pharmacological approach and to investigate its potential mechanism of action. Ultra sonication extraction of Cardiospermum halicacabum leaves was performed, identifying 1294 natural compounds via O-HRLCMS, with 294 compounds screened. Cervical cancer-associated gene targets were retrieved from databases, and their functions with related pathways were examined. Networks were built using Cytoscape v3.7.2, and ligand docking

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was performed with Autodock tools. Swiss ADME and Pre ADMET analysed pharmacokinetic properties. An in vitro study confirmed the anti-cervical cancer activity. Our findings indicate that the anticancer activity of Cardiospermum halicacabum involves 9 compounds and 10 targets, forming significant networks. Molecular docking estimated the binding affinity of protein-ligand complexes, with 19- Nortestosterone showing highest binding affinity (-8.4) than standard with 5F19. The In-vitro study using the HeLa CCL2 cell line demonstrated significant anticancer activity of the extract.

Key Words: Cervical cancer, Cardiospermum halicabum, HeLa CCL2

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Bottom-Up Approach for Carbon Dots Synthesis and its Application as Catalyst to Synthesis of Benzopyran Series.

Rakesh kumar sonka
Amity University, kharora , Raipur
*Email: rakeshsonkar90@gmail.com

Abstract: Carbon dots (CDs), a type of nanostructured carbon material, are created through a simple and cost-effective process known as the bottom-up approach. This involves thermally breaking down or carbonizing molecular precursors like citric acid, carbohydrates, or amino acids. By adjusting reaction conditions, CDs can be tailored to exhibit desirable features such as a high surface area, abundant functional groups, and photoluminescence. These unique properties make them highly adaptable for various applications. In organic synthesis, CDs serve as effective catalysts, particularly in forming benzopyran derivatives. They facilitate multicomponent reactions (MCRs) involving aldehydes, phenols, and active methylene compounds. The catalytic action of CDs stems from their surface functional groups, which activate aldehydes, enhance nucleophilic interactions, and stabilize reaction intermediates through electron transfer. Moreover, their ability to function as photocatalysts under visible light further boosts reaction efficiency. This eco-friendly catalytic system stands out for its improved reaction selectivity, reusability, and non-toxic nature, aligning with the principles of green chemistry. This study underscores the potential of CDs as sustainable nanocatalysts in synthesizing complex organic structures like benzopyrans.

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Synthesis of Coumarin Derivatives

Rathod Dipak Balasaheb, Sonkamble V.S
Research centre in Chemistry, Department of Chemistry, Dayanand Science College, Latur 413512-Maharashtra India
*Email: rss.333@rediffmail.com

Abstract: Coumarin derivatives have gained significant attention due to their wide range of pharmacological activities, including anticoagulant, antiinflammatory, antimicrobial, antioxidant, and anticancer properties. This work focuses on the synthesis of coumarin derivatives through various methodologies, including Pechmann condensation, Knoevenagel condensation, and Claisen

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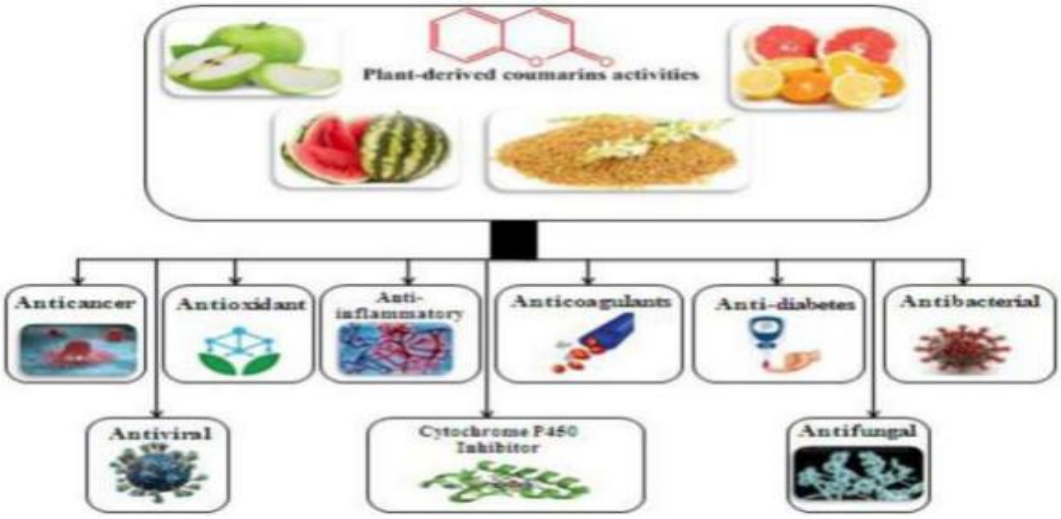
rearrangement.

The optimization of reaction conditions, such as catalyst selection, temperature, and solvent choice, plays a critical role in improving yields and minimizing by-products. Additionally, green chemistry approaches, such as the use of ionic liquids and microwave-assisted synthesis, are explored to enhance sustainability. The synthesized coumarin derivatives are characterized using techniques like NMR, IR, and mass spectroscopy, confirming their structures. This study highlights the potential of coumarin derivatives for applications in drug development and other industrial fields.



Abstract ID: ICCSHIP-2025/A-137

Recent Developments Nanotechnology in Solar Cell

Sunil B. Aute
Kohinoor Arts Commerce and Science College Khultabad, Khultabad, Chhatrapati Sambhajinagar
Email: sbaute9@gmail.com

Abstract: Nanotechnology is fast emerging field in the recent era, in this field nonstop advances and breakthroughs. Numerous nanoscale materials and coatings are already found in consumer goods such Energy, paints, dyes, fibers and textiles, sunscreens, and cosmetics. The smallest components of a computer chip are on a nanoscale. Nanotechnology has demonstrated great potential for energy uses through the manipulation of materials at the molecular level. Distinct optical, electrical, and mechanical characteristics of materials such as perovskite solar cells, Quantum Dot Solar, and dye-sensitized solar cells enable their application in renewable energy generation and pollutant elimination. perovskite solar cells has the maximum power conversion efficiency is 24% that, Quantum Dot Solar has the reported PCE about 12.7%, and Dye sensitized solar cell has the maximum PCE reported as a 13%. The swift rise of the worldwide population has markedly heightened energy usage and strain on the environment.

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Abstract ID: ICCSHIP-2025/A-138

Synthesis and Cytotoxic Evaluation of Bis-difluoromethoxy Curcumin (BDFMC) and Monocarbonyl Analogues of Bis-difluoromethoxy Curcumin (MCAC) as Potential Anti-Cancer Agents

Bhausaheb B. Bhagwat, Mahesh R. Kulkarni, Mahesh B. Dawange, Nitin D. Gaikwad*
Organic Chemistry Research Centre, Department of Chemistry, K.R.T. Arts, B.H. Commerce & A.M. Science College, Gangapur Road, Nashik 422002, MS, India.
Email: bhagwatbhausaheb123@gmail.com

Abstract: In the present study in order to expand the scope of SAR of biologically important natural product Curcumin, novel molecules were designed by displacement of the methoxy group with its bioisostere difluoromethoxy group. Synthesis of the designed Bis-difluoromethoxy Curcumin and monocarbonyl analogues of bis-difluoromethoxy Curcumin were achieved by the multistep reaction sequence (Scheme-2 & 3) with good to moderate yield. Structure of all newly synthesized compound were ascertained by various spectroscopic technique. All synthesised compounds were tested for cytotoxic potential against human breast cancer MCF-7, MDA-MB-231 cell lines and normal monkey renal Vero cell line. From the series majority of the newly synthesised Curcumin derivatives displayed moderate to good in-vitro cytotoxicity. The inhibitor BDFMC (C2), MCAC-8 and MCAC-10 were inhibited MDA-MB-231 cancer cell growth significantly with GI50 of 4.75, 1.51 and 1.46 µM respectively and displayed the significant improved cell viability over the parent Curcumin on the tested cancer cell lines.

Key word: Curcumin, Bis-difluoromethoxy Curcumin (BDFMC), Monocarbonyl analogues of Bis-difluoromethoxy curcumin (MCAC), Cytotoxicity.

Abstract ID: ICCSHIP-2025/A-139

Design, Synthesis, and Biological Study of Quinazoline Derivatives Containing 5-(4-methyl phenyl)-1, 3, 4-Thidiazole Moiety

S. D. Rakhe[1], S. S. Mahurkar[1], S. N. Niwadange[2], B. D. Kamale[1], J. A. Angulwar[1]
[1]Department of Chemistry, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA
[2]Dept. Of Chemistry, Shri Govindrao Munghate Arts and Science College, Kurkheda, Maharashtra,
Email: shreyas.mahurkar@gmail.com

Abstract: The design, synthesis, and biological evaluation of a novel series of quinazoline derivatives containing a 5-(4-methylphenyl)-1, 3, 4-thiadiazole moiety were investigated in this study. The target compounds were synthesized through condensation of isatoic anhydride, aldehyde and 2-amino-(4-methylphenyl)-1, 3, 4-thiadiazole in ethanol using catalyst at reflux condition to form quinazoline derivatives with 5-(4-methylphenyl)-1, 3, 4-thiadiazole. The synthesized compounds were characterized by various spectroscopic techniques, including NMR, IR, and mass spectra, to confirm their structure and purity. The biological activities of the derivatives were evaluated against a range of pathogenic microorganisms, including bacteria and fungi, using standard antimicrobial assays.

Keywords: Isatoic anhydride, aldehyde, quinazoline derivatives, thiadiazole, biological activity.

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Abstract ID: ICCSHIP-2025/A-140

Synthesis of New 1, 2, 3-Triazoles for Their Antimicrobial Evaluation

Sachin J. Khochare, [1,2] Sambhaji T. Dhumal,[2] Tejshri R. Deshmukh,[3] Meghshyam K. Patil,[4] A.W. Suryawanshi[1]*

[1]Department of Chemistry, Shri Madhavrao Patil Mahavidyalaya, Murum Dist. Dharashiv-413605,
[2]Department of Chemistry, Ramkrishna Paramhansa Mahavidyalaya, Dharashiv- 431501,
[3]Sundarrao Solanke Mahavidyalaya, Majalgaon, Dist. Beed-431131, Maharashtra, India
[4]Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University Subcampus, Dharashiv-431501, Maharashtra, India,
Email: surya44444@yahoo.com

Abstract: In search of potent antimicrobial agents, herein we have reported new 1, 2, 3 triazoles from substituted salicylaldehyde by following click chemistry approach. The cycloaddition reaction between key intermediate alkyne of substituted salicylaldehyde and various phenyl azides in the presence of catalyst $CuSO_4$ and sodium ascorbate in PEG-400 as a solvent. All the newly synthesized compounds were thoroughly characterized by 1H NMR, 13C NMR and HRMS techniques. All the newly synthesized compounds were screened for their antimicrobial activity against various antibacterial and antifungal strains. Among the series, some of the compounds were displayed potent antimicrobial activity against pathogenic antibacterial and antifungal strains as compared to the standard reference drug, tetracycline.

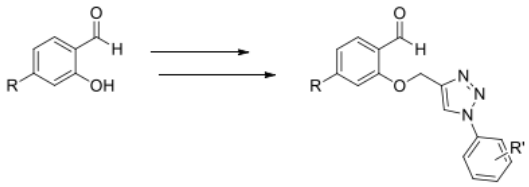

Figure 1. Synthesis of new 1,2,3-triazoles from substituted salicylaldehyde.

Abstract ID: ICCSHIP-2025/A-141

Development, Formulation and Bioactivity Analysis of Advanced Herbal Hair Serum Using Bioactive Plant Extracts from Marathwada

Sachin Ganpatrao Mane
Research center in Chemistry, Department of Chemistry, Dayanand Science College, Latur – 413 512, Maharashtra, INDIA
Email: sm6025302@gmail.com

Abstract: This study emphasizes the development, formulation, and bioactivity assessment of innovative herbal hair serums through the use of bioactive plant extracts from Marathwada, India. Three hair serum batches were developed with different proportions of coconut oil, almond oil, rose water, hibiscus oil, sunflower seed oil (for Vitamin E), and distilled water. Each batch was evaluated

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for physical appearance, odor, homogeneity, pH, and contamination. Furthermore, customer reviews were gathered to determine the effectiveness and acceptability of the formulated hair serums. The outcomes of this study are expected to offer insights into the possibility of using locally derived plant extracts to create effective and natural hair care products.

Keywords: - Herbal hair serum, bioactive plant extracts, local plant extracts

Abstract ID: ICCSHIP-2025/A-142

Synthesis of Aloe Vera Gel and its application in Cosmetics

Sana S.Gadiwan[1], Aakash S.Singare[2], Vidya Aiwale[3], Seema G. Mehatre[4], Nanda S.Korde*
[1]Dayanand Science College, Latur
[2] School of Chemical Sciences, S.R.T.M.University, Nanded
[3]Yogeshwari Mahavidyalaya, Ambajogai
[4]Shri Chhatrapati Shahu Maharaj Sainiki Junior college, Udgir
Email: nandineekorde0@gmail.com

Abstract: Plant-based herbal gel is used in cosmetic products for the treatment of skin. Very commonly include succulent aloevera, which heals, reduces pain and moisturizes to the skin. For hundreds of years, it has healed skin burns and injuries. Aloe vera is used with polymers in gels to provide synergistic effect and moisturizing effect on skin. The utilization of aloe vera, honey and glycerine in the formation of an herbal gel is an exemplary notion. Aloe-vera , Honey were taken by the formulation of herbal skin gel Evaluation parameters were also performed to evaluate the formulation and to make sure that the subjected formulation is not harmful for the human body.The external use of herbal gel in cosmetics primarily acts as skin healer and prevents injury of epithelial tissues, cures acne and gives a youthful glow to skin, also acts as extremely powerful laxative.The herbal gel is useful to treat skin conditions by formulating and evaluating on the basis of pharmaceutical assessment.

Keywords: Herabal Aloe-vera gel, Beauty Skin, Cosmetic application.

Abstract ID: ICCSHIP-2025/A-143

Phytochemical Analysis, in silico and In- Vitro Study of Cynodon Dactylon Leaves Extract for Insecticidal Activity

Kale Dhananjay Damodar
School of Pharmacy SRTMU Nanded 431606
Email: kaledhananjay2001@gmail.com

Abstract: Cynodon dactylon, commonly known as Bermuda grass, is a versatile medicinal plant widely recognized for its phytochemical properties. This study focuses on the phytochemical analysis, in silico evaluation, and in vitro investigation of C. dactylon leaf extract for its potential insecticidal activity. The phytochemical screening revealed the presence of bioactive compounds such as flavonoids, alkaloids, tannins, and phenols, which are known for their pesticidal properties.Pass studies were performed to predict the insecticidal activity. In vitro assays further

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validated the insecticidal activity, showcasing significant mortality rates against selectedspecies. The study highlights the potential of C. dactylon as a sustainable source for the development of eco-friendly insecticides and emphasizes its importance in integrated pest management strategies.

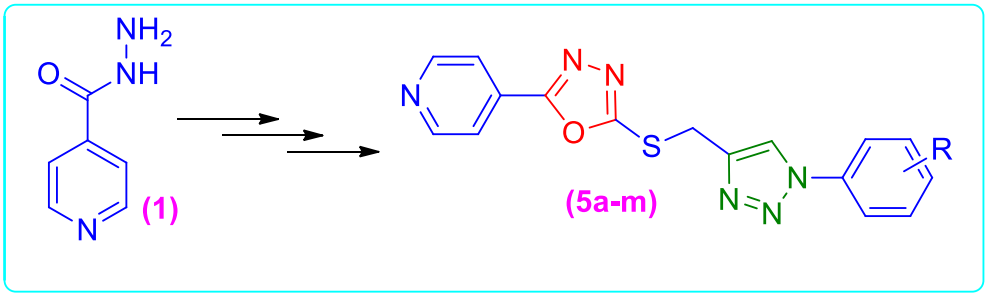
Keywords: Cynodon dactylon, phytochemical analysis, Insecticidal activity, Eco-friendly insecticides, integrated pest management

Abstract ID: ICCSHIP-2025/A-144

Design, Synthesis and Biological Evaluation of Some Novel Oxadiazole-Triazole Molecular Hybrids as Antitubercular Agents

Shriram B. Pawar, Shyam V. Londhe, Kishan P. Haval*
Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar
Sub-Campus, Dharashiv-413501 (MS) India
Email: havalkp@gmail.com

Abstract: In ongoing search toward discovering novel antitubercular drugs, we have designed and synthesized a series of novel oxadiazole-triazole molecular hybrids. The structures of newly synthesized compounds were confirmed by using different spectral techniques such as 1H NMR, 13C NMR and HRMS. Target molecules were further evaluated for their antitubercular potential against M. tuberculosis. The in vitro screening of oxadiazole- triazole hybrids entities offered four potent antitubercular molecules. Our finding indicated that these newly synthesized oxadiazole–triazole molecular hybrids may considered as potent antitubercular drugs against the mycobacterium tuberculosis.



Keywords: Isoniazid, Triazole, Oxadiazole, Antitubercular activity.

Abstract ID: ICCSHIP-2025/A-145

Exploring the Anti- Alopecia Potential of Xanthium Strumarium L.: An Integrated In Vitro and In Silico Study

Shruti Kishor Waikar
School of Pharmacy, Swami Ramanand Teerth Marathwada University, Nanded (431606)
Email: shrutiwaikar278@gmail.com

Abstract: Alopecia is a common medical condition characterized by hair loss, which can occur on the scalp. The research includes morphological traits for exact species identification, physicochemical

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standards for quality assurance, and a wide spectrum of bioactive substances discovered by phytochemical screening. Metabolite profiling highlights its potential in pharmacology, while computational predictions and molecular docking suggest anti-alopecia properties. The binding energies calculated through molecular docking are indicative of the strength of the ligand-receptor interactions. Phytoconstituents with the lowest binding energies in docking studies hold promise for developing anti-alopecia drugs. Enzyme inhibition assays confirm its potential as a natural 5-alpha reductase inhibitor. Collectively, the findings emphasize Xanthium strumarium potential as a therapeutic resource. Total 438 metabolites were identified using OHR-LCMS analysis 19-Nortestosterone have highest pass score and has the potential to treat hair loss. Conduct in silico molecular docking studies to explore compound interaction with hair related protein. As research continues, Xanthium strumarium stands as promising botanical asset with multifaceted benefits. The potential of Xanthium strumarium anti-alopecia source has been suggested by computational models, but experimental confirmation is necessary for practical use. Diverse bioactive compounds identified through phytochemical screening, such as alkaloids and flavonoids, highlight Xanthium strumarium therapeutic potential, encouraging further exploration. Molecular docking studies reveal compounds like 19- nortestosterone as potential leads.
Keywords: Alopecia, molecular docking, 19- nortestosterone, Xanthium strumarium

Abstract ID: ICCSHIP-2025/A-146

Sound Pollution Control System for Environment Safety Using WSN and IoT

R. B. Shinde, T. H. Mujawar
[1]Department of Computer Science, Dayanand Science College, Latur
[2]Department of Electronics, Dayanand Science College, Latur
Email: rvmali007@gmail.com

Abstract: Sound is very important for communication but when we think about the sound which create noise, it adversely effects on environment & affecting on living things. It also effects on human beings. Due to sound pollution Hearing Impairment, Cardiovascular issues, Sleep disturbances, Mental Health effect, Development Issues in Children occurs. As this Civilization increases the noise pollution increases as well. It is very important to think the sound pollution which is not visible but gives very severe effect on environment. The proposed system work on Causes of sound pollution, data collection from different areas where sound pollution occurs & and gives the alertness were sound pollution increases. Urbon locations such as Hospitals, Schools, and Industrial districts, as well as some sensitive places, will get benefit from this proposed system. In order to continuously monitor the noise levels across multiple sites, this system will install sound sensors in scattered areas. These sensors will gather data in real time and send to server it over a Wi-Fi network. Where it is possible to analyse sound pollution data and patterns of sound pollution. Proposed system gives alert to users when noise levels increase above a predefined threshold and to prompt appropriate action. The system is a vital tool for environmental authorities and urban planners to efficiently control and minimize noise pollution since it uses IOT technology for scalability, flexibility, and remote accessibility.
Keywords: MEMS, Integrated Noise Sensors, Condenser Microphones, and IoT etc.

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Abstract ID: ICCSHIP-2025/A-147

Synthesis and Biological Evaluation of Some Heterocyclic Compounds

Komal Doifode*, Dr. Shailaja Jadhav
PES's Modern College of Pharmacy Nigdi, Pune 44
Email: komaldoifode775@gmail.com

Abstract: The 7-azaindoles shows lot of biological activities such as analgesic, anticancer, Rho-kinase inhibitor, Thrombin inhibitor, Antibacterial activity etc. A series of four 7-azaindole derivatives 6a-6d were synthesized and evaluated for antimicrobial activity. The compound 6a and 6d have shown excellent activity and 6c have shown equal potency as that of standard drug Azithromycin against gram negative bacteria (P. aeuginosa).

Keywords: Analgesic, Anticancer, Antibacterial, Antifungal, Heterocyclic.

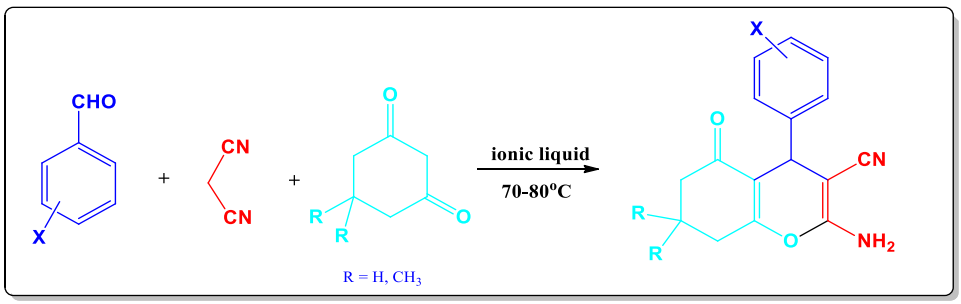
Abstract ID: ICCSHIP-2025/A-148

Ionic liquid-Mediated One-Pot Three Component Synthesis of 2-Amino- 4H-Chromene Derivatives

Tukaram Khatke [1], Shreyas Mahurkar[2], Sangita Makone[3]*
[1]Department of Chemistry, NKSPT Arts, Science & Commerce College, Badnapur-431202, India
[2]Department of Chemistry, Dayanand Science College, Latur-413512, India
[3]School of Chemical Sciences, SRTMU Nanded -431606, India.
Email: ss_makone@rediffmail.com

Abstract: In this study, we report an imidazolium ionic liquid-mediated approach for the one-pot, multi-component synthesis of 2-amino-4H-chromene derivatives. The reaction involves the condensation of aromatic aldehydes (1), malononitrile (2), and dimedone/1,3-cyclohexanedione under green, environmentally friendly conditions. The structure of the synthesized products was confirmed using FT-IR, 1H NMR, and 13C NMR spectroscopy. This method offers several advantages, including ease of preparation, short reaction times, high yields, and simple work-up procedures.

Keywords: Aldehyde, malanonitrile, dimedone/1,3-cyclohexanedione, ionic liquid, 2-amino-4H-chromene



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Abstract ID: ICCSHIP-2025/A-149

Review on Soil and Agriculture Chemistry

Ustad S.F, D.K. Borolkar, Ustad. H.F., Muley D. B.
Chemistry Department, PG students, shivaji Mahavidyalaya, Udgir (MH)-413512
Email: kamalustad846@gmail.com

Abstract: Agricultural management is a key force affecting sol processes and functions. Triggered by biophysical constraints as well rapid structural and technological developments, new management practices rging with largely unknown impacts and functions. This nts of the potential of tices for sustainable soil impedes such emer intensification, paradigm coined to address the growing demand for food and nonfood.products. In terms of soil management, sustainable intensification means that soil productivity is increased while other soil functions and services, such as carbon storage and habitat for organisms. Are simultaneously maintained or even improved. In this paper we provide an overview of research challenges to better understand how emerging soil management practices affect soil processes and functions.

Abstract ID: ICCSHIP-2025/A-150

Determination of the Dissociation Constant of an Organic Acid By pH Metrically.

Patil Vrushali Sandeep
Dayanand Science College, Latur
Email: patilvrushali055@gmail.com

Abstract: Acids and bases play a significant role in many areas of chemistry and biochemistry. We can classify substances as acids and bases based on chemical behavior. Acetic acid being a weak acid. It is partially dissociated in aqueous solution and sodium acetate is a salt of weak acid and strong base. Various buffer's solutions can be prepared by mixing acid solution in the solution of its salt in different proportions. The pH value depends upon the proportion of these two substances. The determination of the acid dissociation constant is an important step in the development of new pharmaceutical products since this physico-chemical parameter can strongly affect product efficacy. The pKa value value indicates the strength of an acid in a specific solvent. This quantity is not only important for the classification of an acid, but also determines the properties of a substance in nature or its possible use as a drug. The determination of the pKa value is therefore of great importance in the pharmaceutical and agrochemical industries. In drug research, synthesized compounds are screened for their ability to interact with specific target sites in biological entities such as enzymes, proteins, or cells. Only those compounds that show the desired biological activity, i.e. which are successfully absorbed and transferred to the target sites, are promising candidates for new drugs in medical therapy. Almost all drug molecules form ionized species in aqueous solutions through the release of hydrogen ions H+. Due to the relationship between pKa and pH, the pKa indicates which form of a drug molecule will exist at a given pH.

Keyword: Weak acid, pH meter, pKa, dissociation constant

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Abstract ID: ICCSHIP-2025/A-151

Synthesis, Structural, Morphological and Optical Properties of Cd-Doped Zns Nanoparticles Via Co-Precipitation

Y. S. Sudake[1]*, [2]S.D. Lokhande, V. D. Mote[2]
[1]Dept. of Physics, New Arts, Commerce and Science College Shevgaon-414502 Maharashtra, India
[2]Thin Film and Materials Science Research Laboratory, Department of Physics, Dayanand Science College, Latur-413512, Maharashtra, India.
Email: ysudake@gmail.com

Abstract: Undoped and Cd-doped ZnS nanoparticles have been synthesized via the chemical co-precipitation technique. The morphological, structural and optical properties of the nanoparticles have been investigated by scanning electron microscope (SEM), x-ray diffraction (XRD) and UV-Vis spectrophotometry. SEM micrographs indicate that the obtained nanoparticles consist of spherical like shape of particles. The XRD patterns confirm the prepared samples have cubic crystal structure. The lattice constant of ZnS was increase with increasing Cd doping concentration. In addition, the volume of unit cell increases with increasing Cd doping was observed. The average crystallite size was found to be in the range of 2.1 to 3.2 nm of Cd doped samples. The optical properties of ZnS and Cd-opded ZnS samples were systemically inverigated and reported in this paper. Based on the structural and optical studied the prepared Cd-doped ZnS nanoparticles can be promising materials for opto-electronics application.
Keywords: Semiconductor; nanoparticles; Cd-ZnS; SEM; strain, optical properties.

Abstract ID: ICCSHIP-2025/A-152

Review on Nano Science and Material Chemistry

Zarger Bushra A.S.A, Tekale A.S, Reddy P.S., Muley D.B
Chemistry Department, PG Student in Shivaji Mahavidyalaya Udgir, (MH) - 413517
Email: zargerbushra@gmail.com

Abstract: This paper presents comprehensive study of nano materials and nanotechnology, encompassing synthesis methodologies, advanced characterization techniques and diverse applications. Nanomaterials, engineered at the nanoscale, exhibit unique properties and hold immense promise for revolutionizing various industries. The study covers five key subheadings, addressing synthesis approaches, characterization methods, and multifaceted applications in medicine, energy, electronics and future prospect in the field. The core of this comprehensive study devels into the multifaceted applications of nanomaterials covering a broad spectrum of fields ranging from medicine and pharmaceuticals to envionrnmental science and renewable energy. The unique properties of nanomaterials, such as increased surface area and reactivity are shown to enhance the efficacy of drugs and treatment methods. The interdisciplinary nature of nanomaterials and their vast potential make this field a cornerstone of future advancements in science and engineering
Keywords: Nanomaterials, Nanotechnology, Synthesis, Characterization, Multifaceted applications, Future prospects

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Abstract ID: ICCSHIP-2025/A-153

Synthesis, Characterization and Biological Studies of Schiff Bases Derived from DHA and Primary Amines

Apurva Bhalekar, Pruthviraj Chauhan, D. G. Palke*.
Department of Chemistry, Rajarshi Shahu Mahavidyalaya, Latur
Email: dhananjaypalke@gmail.com

Abstract: The coloured solid DHA Schiff base ligand derived from Dehydroacetic Acid and aromatic primary amine 3,4-dichloro aniline, 2-amino pyridine, 3-amino pyridine and 4-amino-1,2,4-triazole were synthesized, characterized by elemental analysis, Spectroscopic techniques (FTIR, UV-VIS, and 1HNMR), and Investigated For Anti-bacterial and Anti-fungal biological activities. DHA Schiff base ligands were screened in vitro against Bacillus subtilis, Staphylococcus aureus, Aspergilus niger and Candida albicans. The structure of synthesized DHA Schiff base ligands were confirmed by spectroscopic methods, DHA Schiff base ligands are strongly active against bacteria and fungi.
Keywords: Dehydroacetic Acid, Primary Amines Schiff Bases, Biological Activity.

Abstract ID: ICCSHIP-2025/A-154

Innovations in Chemical Analysis: The Power of Hyphenated Techniques

Manisha Bhattacharya
Ramniranjan Jhunjhunwala College, Ghatkopar (W) Mumbai.
Email: manishab44@gmail.com

Abstract: Hyphenated techniques have revolutionized chemical analysis by integrating separation and detection methods to achieve higher sensitivity, specificity, and efficiency. These techniques, such as GC-MS, LC-MS, HPLC-NMR, and ICP-MS, provide comprehensive insights into complex samples across diverse fields, including pharmaceuticals, environmental science, food safety, and forensic analysis. The interface between components plays a crucial role in ensuring seamless sample transfer, maintaining resolution, and enabling efficient ionization for accurate detection. Innovations such as advanced ionization methods, miniaturization, artificial intelligence-driven data interpretation, and green analytical approaches continue to enhance the power and applicability of hyphenated techniques. Despite challenges like high costs and complex data analysis, the future of chemical analysis will be shaped by continuous advancements in multi-hyphenation, automation, and real-time analytical capabilities. This talk explores the principles, innovations, applications, and future prospects of hyphenated techniques, highlighting their impact on modern analytical chemistry.

Abstract ID: ICCSHIP-2025/A-155

Recent Advances and Future Perspectives in Spinel Ferrite Research: Synthesis, Characterization, and Applications

Jairam B. Mote
Department of Chemistry, Adarsh College, Omerga, Osmanabad, Maharashtra, India
Email: jbmote51172@gmail.com

Abstract: Spinel ferrites, a versatile class of magnetic materials with the general formula AB2O4, have attracted significant research interest due to their unique combination of electrical, magnetic, and catalytic properties. Their wide-ranging applications in electronics, data storage, biomedicine, and energy technologies underscore their immense technological and industrial significance. The

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historical development of spinel ferrites traces back to the early 20th century, with major breakthroughs in synthesis and applications emerging over the decades. Conventional techniques such as solid-state reaction and wet chemical methods have evolved into advanced nano structuring approaches, enabling precise control over material properties. Characterization techniques, including X-ray diffraction (XRD), electron microscopy (TEM/SEM), and magnetic measurements (VSM, SQUID), are essential for understanding phase purity, microstructure, and magnetic behavior. Recent advances in spinel ferrite research have focused on tailoring their properties for enhanced performance in energy storage, environmental remediation, and biomedicine. However, challenges such as scalability, cost-effective synthesis, and stability under operational conditions remain key concerns. Future research directions emphasize optimizing synthesis techniques, developing multifunctional ferrites, and exploring new frontiers in quantum and spintronic applications. This review provides a comprehensive analysis of the latest progress in spinel ferrites, highlighting their synthesis, characterization, applications, and future prospects. The insights presented herein aim to guide researchers toward addressing existing challenges and expanding the potential of spinel ferrites in advanced technological applications.

Keywords: Spinel Ferrites, Magnetic Materials, Synthesis, Characterization, Applications.

Abstract ID: ICCSHIP-2025/A-156

A Study of Some Heterocyclic Compounds Moeity with Respect To 2, 4, 5-Triphenyl Imidazole for Synthesis and Characterisation

Pathan Farida Parvez
Rajarshi Shahu Mahavidyalaya, Latur - 413512
Email: faridapathan226@gmail.com

Abstract: The FT-IR and FT-Raman spectra of 2-(4-Methoxyphenyl)-4, 5-diphenyl1H-imidazole (MPDPI) molecule have been recorded in the region 4000-400 cm-1 and 3500-100 cm-1 respectively. Optimized geometrical structure, harmonic vibrational frequencies, and intensities have been computed by the B3LYP density functional levels using ccpVDZ and 6-311G basis sets. The observed FT-IR and FTRaman vibrational frequencies are analyzed. The geometries and normal modes of vibration obtained from DFT method are in good agreement with the experimental data. The charge transfer occurring in the molecule between HOMO and LUMO energies, frontier energy gap, the molecular electrostatic potential (MEP) were calculated and analyzed.

Abstract ID: ICCSHIP-2025/A-157

Unraveling Physical Chemistry Underlying Drug DNA Interaction

Palak Chawla
Ramniranjan Jhunjhunwala College, Mumbai -86
Email: palakchawla@rjcollege.edu.in

Abstract: The interaction between drugs and DNA plays a crucial role in the development of therapeutics, particularly in anticancer and antibiotic treatments. Physical chemistry provides a fundamental understanding of these interactions by exploring thermodynamics, kinetics, and molecular binding mechanisms. This study reviews key principles such as hydrogen bonding, π–π stacking, electrostatic forces, and van der Waals interactions that govern drug-DNA binding.

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Experimental techniques, including spectroscopy, calorimetry, and molecular docking simulations, are discussed in relation to their role in characterizing binding affinity and specificity. Additionally, the impact of DNA conformation and drug physicochemical properties on interaction strength is highlighted. Understanding these principles aids in rational drug design, optimizing drug efficacy while minimizing off-target effects.

Abstract ID: ICCSHIP-2025/A-158

Clinical Trials: The Transition from Traditional To In- Silico Approaches

Vishal Wadekar*, Aachal Mulgir
Shivlingeshwar college of pharmacy, almala, Latur, Maharashtra, India -413520
Email: wadekarvishal162@gmail.com

Abstract: The term 'in silico clinical trials' refers to the development of patient-specific models to form virtual cohorts for testing the safety and/or efficacy of new drugs and of new medical devices. Moreover, it could be envisaged that a virtual set of patients. In Silico trials or virtual clinical trial is a computer stimulation used in drug development. It uses AI to create virtual models of human physiology based on real world clinical data and stimulate their response to various medical interventions. Its aim is to refine, reduce and may replace traditional clinical trials which are often costly, time consuming and ethically challenging also enable personalized medicine by adjusting the treatment to the specific characteristics of each patient.
Keywords: Clinical trials, statistical data, drug development, accuracy, ethical concerns, cost effectiveness.

Abstract ID: ICCSHIP-2025/A-159

Facile Hydrothermal Synthesis of Carbon Dots from Caesalpinia crista L. Leaves and Their Characterization

Rajesh Valvi[1], Anil Athare[1]*, Sushama Takate[2]
[1]Department of Chemistry, New Arts, Commerce and Science College, Shevgaon Dist. Ahmednagar, Maharashtra- 414502, India.
[2]Department of Chemistry, New Arts, Commerce and Science College, Ahmednagar, Maharashtra- 414001 India
Email: ltanilathare@gmail.com

Abstract: Plant-derived carbon dots (CDs) have attracted considerable attention due to their multifunctional surface, biocompatibility, low toxicity and multiple applications in medical and other fields. **Objective:** To provide the first report on CDs derived from CCL leaves and analyze their structural, morphological and spectroscopic properties. **Method:** The present synthesis work utilizes the leaves of CCL to synthesize CDs through easy and simple hydrothermal method. The synthesized CDs were characterized using ultra violet-visible (UV-Vis), Fourier transform infrared (FT-IR) and Raman spectroscopy, in combination with X-ray diffraction (XRD), High resolution transmission emission microscope (HR-TEM) and elemental analysis. **Result:** The UV-Vis spectra of CDs exhibits two maximum absorption peaks at 227.7 nm and 379.4 nm, while the FT-IR spectrum identifies a vibrational frequencies of bonds at 3350, 1712, 1620 and 1070 cm^{-1}. Raman

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spectroscopy shows the D and G bands are at 1354 cm^{-1} and 1594 cm^{-1}, respectively. The XRD analysis reveals prominent peaks at 28.3° and 40.5°, while the HR-TEM and selected area electron diffraction (SAED) images confirm the formation of quasi-spherical, uniformly distributed and amorphous CDs with an average particle size of 7.9 nm. Elemental analysis finding indicate that the carbon was predominant component followed by oxygen, hydrogen and nitrogen. **Conclusion:** The leaves of CCL can be used as a green precursor for the synthesis of CDs by hydrothermal methods with average size 7.9 nm and UV-Vis, FT-IR, Raman spectroscopy, XRD, HR-TEM and elemental analysis as fundamental characterization techniques.

Abstract ID: ICCSHIP-2025/A-160

Nanotechnology and SNEDDS: Revolutionizing Pharmaceutical Sciences and Drug Delivery

Maithili Kamble, Amrapali Rajput, Rudranee Wagdare
Department of Pharmaceutics, Channabasweshwar Pharmacy College (Degree), Latur, Maharashtra, India-413512
Corresponding email: maithilikamble7@gmail.com

Abstract: In pharmaceutical sciences, nanoscale carriers are explored to enhance drug performance by improving solubility, permeability, drug distribution, and stability in physiological environments.. This study specifically investigates SNEDDS for the topical administration of 5-Fluorouracil (5-FU), an anticancer agent for treating skin conditions like actinic keratosis and basal cell carcinoma. SNEDDS are isotropic mixtures of oils, surfactants, and co-surfactants that form nano-sized emulsions upon dilution, significantly enhancing drug solubility, stability, and transdermal permeability. Using both high-energy and low-energy emulsification techniques, SNEDDS formulations were systematically developed. The optimized SNEDDS was integrated into a topical cream and evaluated for drug content, entrapment efficiency, self-emulsification time, spreadability, viscosity, in-vitro drug release. Results indicated a viscosity range of 1532–5273 cP, spreadability-5.866-6.354 drug content between 38.43% and 52.32%, and entrapment efficiency from 60.41% to 77.06%. The findings demonstrated notable improvements in 5-FU's solubility, stability, and skin penetration, validating the potential of this innovative SNEDDS-based topical cream for effective treatment of skin cancers. This approach offers a promising strategy for advancing transdermal drug delivery systems, providing enhanced therapeutic outcomes and improved patient compliance.

Keywords: Nanotechnology, SNEDDS, Topical drug delivery, 5-Fluorouracil, actinic keratosis, targeted therapy, diagnostics, emulsification techniques, therapeutic efficacy.

Abstract ID: ICCSHIP-2025/A-161

Synthesis of Fused Benzotriazole Derivatives by Microwave Irradiation

Pawan More, Ganesg Jadhav, Ganesh Vaidya, Maroti Sudewad*
Department of Chemistry & Analytical Chemistry, Rajarshi Shahu Mahavidyalaya, Latur, Maharashtra, India-413512
Corresponding email: maithilikamble7@gmail.com

Abstract: Triazole is a nitrogen-containing heterocyclic compound. Triazoles contain Three nitrogen atoms and two carbon atoms and are divided into two isomers, that is 1,2,3-Triazole and 1,2,4-Triazole.Triazoles and their derivatives have important biological properties such as

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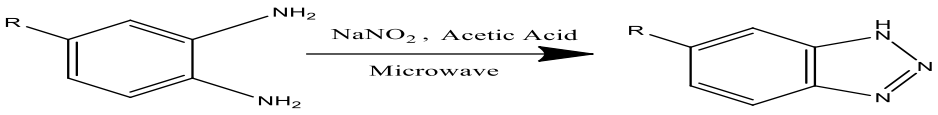
antibacterial, antiviral, anti-tuberculous, anticancer, anticonvulsant,analgesic, antioxidant, anti-inflammatory, and antidepressant activities. In this study, we synthesized new, biologically active benzotriazole derivatives using green Approach.



Abstract ID: ICCSHIP-2025/A-162

Photochromism Fluorescence in a Keggin type polyoxometalates and Anthranilic acid in different media.

Pravin Mahadev Kadam
Khare Dhere Bhosale College, Guhagar Tal. Guhagar Dist. Ratnagiri 415703.
*Email: pravinkadam664@gmail.com

Abstract: The photophysical properties of a Keggin-type polyoxometalates (POM) bounded to Anthranilic acid have been investigated. An organic-inorganic hybrid species of a Keggin type polyoxometalates $K_5[Co^{III}W_{12}O_{40}]$ has been synthesized and characterised by various spectroscopic techniques X-ray diffraction analysis, IR analysis, NMR spectra. The florescent aromatic hydrocarbons like Anthranilic acid and cobalt polyoxometalates studies reveals that both closed and open forms are emissive with distinct spectral properties.

Abstract ID: ICCSHIP-2025/A-163

Fabrication of Novel Fluorescent Heterocyclic Motifs for Sensing

Ajinkya R.Pawar , Mahesh P. Pawar*,
Department of Chemistry, Rajarshi shahu mahavidyalaya (Autonomous) Latur-413512, Maharashtra, India
*Email: pawarajinkya730@gmail.com

Abstract: In the present work, we have synthesized (2-(3,5-di-tert-butyl-2-hydroxyphenyl)-1H-benzo[d]imidazol-6-yl)(phenyl)methanone by a simple condensation method. TLC also verifies the formation of the key product and the optimized solvent system ration found is (n-hexane : Ethyl Acetate, 85:15). After recrystallization the spectral analysis of the key compound was carried out and was found in harmony with the predicted structure. The Thermogravimetric Analysis (TGA) curve has shown ~86.59 % decomposition at 355 oC The compound was dissolved in chloroform and has shown green fluorescence under UV light. Further, this compound will be studied for its chemosensing profiling for anions.

Key Words: fluorescent, heterocyclic motifs, sensing, Thermal analysis.

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Abstract ID: ICCSHIP-2025/A-164

NANOSCIENCE &MATERIALS CHEMISTRY

Pooja P. Kharosekar, Pooja.D. Mali, Ankita S. Gadhave
Department of Pharmaceutics M. Pharmacy Shivlingashvar College of Pharmacy, Almala, Latur-413512, Maharashtra, India
*Email: poojakharosekar22@gmail.com

Abstract: Material chemistry is a multidisciplinary field that studies the properties &behavior of materials at the nanoscale or billion of materials at the combine chemistry. the impact of nanoscience emerging, the impact of nanoscience emerging science of objective that are intermediate in size between the largest molecules & smallest structure that can be fabricated by photolithograpy on future technology is discussed nanoscience contribute to almost every field of science including physics material sciencer chemistry, biology

Key Words: Nanomaterial, surface chemistry, carbon nanotubesnanoscale.

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Carbon Nanotubes: Applications in Pharmacy and Medicine

Mukhedkar Swanand Shrinivasrao,[1]Deshmukh Jitendra Hanmantrao[2]
[1]Department of Chemistry, Shahir Annabhau Sathe Mahavidyalaya Mukhed.
[2]Department of Chemistry, Mahatma Basweshwar Mahavidyalaya, Latur (MS)
Email: swanandmukhedkar@gmail.com

Abstract

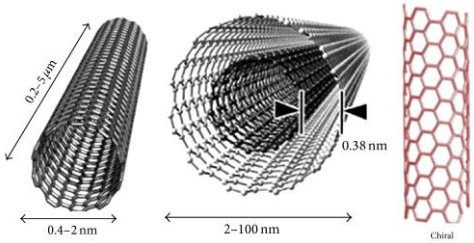
Carbon nanotubes (CNTs) are allotropes of carbon, made of graphite and constructed in cylindrical tubes with nanometer in diameter and several millimeters in length. Because of their structural, mechanical, and electronic properties are due to their small size and mass, strong mechanical potency, and have high electrical and thermal conductivity. CNTs have been successfully applied in pharmacy and medicine due to their high surface area that is capable of adsorbing or conjugating with a wide variety of therapeutic and diagnostic agents (drugs, genes, vaccines, antibodies, biosensors, etc.It works as drug delivery directly into cells without metabolism by the body. Then CNTs have been useful in drug and gene therapies but also for tissue regeneration, biosensor diagnosis, enantiomer separation of chiral drugs, extraction and analysis of drugs and pollutants. Moreover, CNTs have been recently act as antioxidant. It also examines the pharmacokinetics, metabolism and toxicity of different forms of CNTs and discusses the perspectives, the advantages and the obstacles of this promising bio nanotechnology in the future.

1. Introduction

Carbon nanotubes (CNTs), first investigated by Japanese scientist Iijima in 1991 [1], It is used in various industrial areas. These nanomaterials are allotropes of carbon, made of graphite, and have been constructed in cylindrical tubes with nanometer scale in diameter and several millimeters in length [2, 3]. Their impressive structural, mechanical, and electronic properties are due to their small size and mass, their incredible mechanical strength, and their high electrical and thermal conductivity [4, 5]. Carbon nanotubes have been first used as additives to various structural materials for electronics, optics, plastics, and other materials of nanotechnology fields. Since the beginning of the 21st century, they have been introduced in pharmacy and medicine for drug delivery system in therapeutics. Thanks to their high surface area, excellent chemical stability, and rich electronic polyaromatic structure, CNTs are able to adsorb or conjugate with a wide variety of therapeutic molecules (drugs, proteins, antibodies, DNA, enzymes, etc.). They have been proven to be an excellent vehicle for drug delivery by penetrating into the cells directly and keeping the drug intact without metabolism during transport in the body [2–5]. Many studies have demonstrated that when bonded to CNTs, these molecules are delivered more effectively and safely into cells than by traditional methods [3–5].

2. Carbon Nanotubes: Structures, Types and Preparation

Carbon nanotubes (CNTs) consist exclusively of carbon atoms arranged in a series of condensed benzene rings rolled up into a tubular structure. This novel artificial nanomaterial belongs to the family of fullerenes, the third allotropic form of carbon along with graphite and diamond which are both natural sp2 (planar) and sp3 (cubic) forms, respectively [2, 3, 7]. Based on the number of layers, structures of CNTs are classified into two types: single-walled carbon nanotubes (SWCNTs) and multiwalled carbon nanotubes (MWCNTs) (Figure 1).

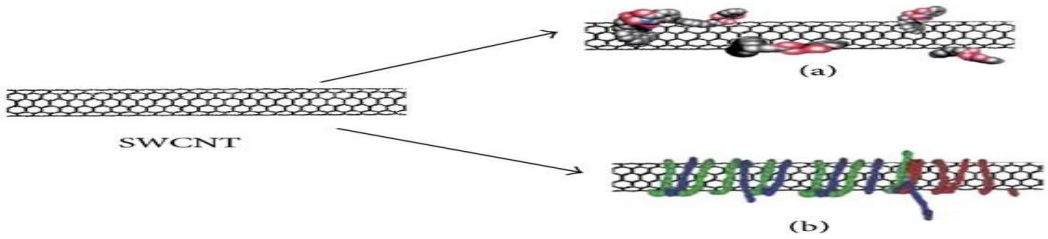


Three main techniques generally used for SWCNTs and MWCNTs production are: Arc-Discharge method (using arc-vaporization of two carbon rods), Laser Ablation method (using graphite), and Chemical Vapor Deposition (using hydrocarbon sources: CO, methane, ethylene, acetylene). After preparation, CNTs are submitted to purification by acid refluxing, surfactant aided sonication, or air oxidation procedure in order to eliminate impurities such as amorphous carbon, fullerenes, and transition metals introduced as catalysts during the synthesis [3, 4, 26]. Pristine CNTs are now synthesized and marketed by many chemical firms worldwide.

3. Carbon Nanotubes: Functionalization for Biomedical Applications

Pristine CNTs are not soluble in aqueous solutions because they have highly hydrophobic surfaces. Surface functionalization is required to solubilize CNTs, and to render biocompatibility and low toxicity for their medical applications [25]. The functionalization procedure of CNTs can be divided into two main approaches, depending on the nature of the biomolecule linked to carbon nanotube, that is, covalent attachment (chemical bond formation) and noncovalent attachment (physioadsorption) [5, 27].

The covalent functionalization of CNTs is generally obtained by oxidation with strong acids (HNO_3). During the process, carboxyl (–COOH) groups are formed at the open sides (tips) and at the defects on the sidewalls of SWCNT or MWCNT, then, further covalent conjugation with amino acid. For the creation of –COOH on the sidewalls of CNTs, nitrene cycloaddition, arylation using diazonium salts or 1,3-dipolar cycloadditions are usually employed [5–7, 27]. Schematic noncovalent functionalization of CNTs is illustrated in Figure 2



4.1. Carbon Nanotubes Used for Cancer Therapy

4.1.1. By Drug Delivery

CNTs can be used as drug carriers to treat tumors [8, 24]. The efficacy of anticancer drugs used alone is restrained not only by their systemic toxicity and narrow therapeutic window but also by drug resistance and limited cellular penetration. Because CNTs can easily across the cytoplasmic membrane and nuclear membrane, anticancer drug transported by this vehicle will be liberated in situ with intact concentration and consequently, its action in the tumor cell will be higher than that administered alone by traditional therapy. Thus, the development of efficient delivery systems with the ability to enhance cellular uptake of existing potent drugs is

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needed. The high aspect ratio of CNTs offers great advantages over the existing delivery vectors, because the high surface area provides multiple attachment sites for drugs [18].
Many anticancer drugs have been conjugated with functionalized CNTs and successfully tested in vitro and in vivo such as epirubicin, doxorubicin, cisplatin, methotrexate, quercetin, and paclitaxel

4.1.2. By Antitumor Immunotherapy

The CNTs used as carriers can be effectively applied in antitumor immunotherapy [3, 26]. This therapeutic consists of stimulating the patient's immune system to attack the malignant tumor cells. This stimulation can be achieved by the administration of a cancer vaccine or a therapeutic antibody as drug. Some authors have validated the use of CNTs as vaccine delivery tools [33]. Yang's group observed that the conjugate of MWCNTs and tumor lysate protein (tumor cell vaccine) can considerably and specifically enhance the efficacy of antitumor immunotherapy in a mouse model bearing the H22 liver tumor [27]. In vitro, the conjugate of CNTs and tumor immunogens can act as natural antigen presenting cells (such as mature dendritic cells) by bringing tumor antigens to immune effector T cells; this action is due to the high avidity of antigen on the surface and the negative charge.

4.1.3. By Local Antitumor Hyperthermia Therapy

The hyperthermia therapy using CNTs has been recently suggested as an efficient strategy for the cancer treatments. SWCNTs exhibit strong absorbance in the near-infrared region (NIR; 700–1100 nm). These nano-materials are considered as potent candidates for hyperthermia therapy since they generate significant amounts of heat upon excitation with NIR light [29–31]. The photothermal effect can induce the local thermal ablation of tumor cells by excessive heating of SWCNTs shackled in tumor cells such as pancreatic cancer. Some progress in the technique has been achieved in recent years, and it has shown feasibility in clinical applications.

4.1.4. Carbon Nanotubes for Neurodegenerative Diseases and Alzheimer Syndrome

As a promising biomedical material, CNTs have been used in neurosciences [3, 5, 24, 36]. Because of their tiny dimensions and accessible external modifications, CNTs are able to cross the blood-brain barrier by various targeting mechanisms for acting as effective delivery carriers for the target brain.

Carbon Nanotubes as Antioxidants:

The theory of oxygen-free radicals has been known about fifty years ago. However, only within the last two decades, has there been an explosive discovery of their roles in the development of diseases, and also of the health protective effects of antioxidants [37]. Nevertheless, the potential role of CNTs as free-radical scavengers is still an emerging area of research.

Carbon Nanotubes for Enantioseparation of Chiral Drugs and Biochemical:

In pharmaceutical industries, 56% of the drugs currently in use are chiral products and 88% of the last ones are marketed as racemates consisting of an equimolar mixture of two enantiomers are separated. microcolumn packed with SWCNT as chiral selector for separation of carvedilol enantiomers, a *β*-blocker, with fluorescent detection.

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Conclusions:

This minireview reveals many spectacular benefits of carbon nanotubes during their recent applications in different areas of pharmacy and medicine. The discovery of this bio nanotechnology has opened new alternatives more effective than the ancient drug delivery methods since CNTs can pass through cell membranes, carrying drugs, genes, biomolecules, vaccines, and so forth deep into the target cells or organs previously unreachable. Another novel approach is the use of collagen CNTs materials as scaffolds in tissue generation and artificial implants because CNTs resist biodegradation and are a powerful engineering candidate over other existing materials used to repair defective organs. Besides, CNTs combined with biosensors or other materials have proven excellent implements for the therapeutic monitoring and the diagnosis of diseases as well as for the analysis of drugs in different areas.

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Review on Nano Science and Material Chemsitry

Zarger Bushra A.S.A, Tekale A. S, Reddy P.S., Muley D.B
Chemistry Department, PG Student in Shivaji Mahavidyalaya Udgir,(MH)-413517
Email: zargerbushra@gmail.com

Abstract

This paper presents comprehensive study of nano materials and nanotechnology, encompassing synthesis methodologies, advanced characterization techniques and diverse applications. Nanomaterials, engineered at the nanoscale, exhibit unique properties and hold immense promise for revolutionizing various industries. The study covers five key ubheadings, addressing synthesis approaches, characterization methods, and multifaceted applications in medicine, energy, electronics and future prospect in the field. The core of this comprehensive study devels into the multifaceted applications of nanomaterials covering a broad spectrum of fields ranging from medicine and pharmaceuticals to envionrnmental science and renewable energy. The unique Properties of nanomaterials, such as increased surface area and reactivity are shown to enhance the efficacy of drugs and treatment methods. The interdisciplinary nature of nanomaterials and their vast potential make this field a cornerstone of future advancements in science and engineering.

Keywords: Nanomaterials, Nanotechnology, Synthesis, Characterization, Multifaceted applications, Future prospects

1. Introduction

Over the last century nanotechnology branch is flourishing to a great extent. And today many types of research are directly or indirectly related to the nanotechnology. Nanotechnology can be stated as the developing, synthesizing, characterizing and application of materialsand devices by modifying their size and shape in nanoscale" In each and every stream the prefix "nano" is using as a keyword even in advertising the products also. Actually the word "nano" is derived from the Greek word nanos or Latin word nanus means which "dwarf". It is the combination of physics, chemistry, material science, solid state, and biosciences. So profound knowledge in one field will not be sufficient, the combined knowledge of physics, chemistry, material science, solid state, and biosciences is required. The applications of Nanotechnology are spreading in almost all the branches of science and technology. The difference between the nanoscience and nanotechnology is the nanoscience gives the knowledge about the arrangement of atoms and their basic properties at nanoscale whereas the nanotechnology is the technology used in governing the matter at the atomic level for the synthesis of the novel nanomaterials with different characteristics [1]. The nanotechnology getting attention in almost all engineering branches but the common people didn't get the knowledge about its existence in daily life but its vast usage in the medicine, engineering, environment, electronics, defense, and security is still increasing (Fig. 1). Even though so much work was done using thistechnology but still have space for developing the new novel nanomaterials in various fields for the progress of mankind. The researchers are fascinated and working for the progress of knowledge in terms of their size, capability, and expenditure. So special interest on the miniaturization othe device with economical is focusing mainly in the field of medicine, electronics. In upcoming days the nanotechnology controls mankind in living,working and communicating fields. So this gives interest in this subject and leads to the discussion of the basic and major topics of nanotechnology. The basic and the key elements of nanotechnology are the "nanomaterials". The nanomaterials are the materials with less than 100 nm size ones at least in one dimension. That means they have very less size than that of microscale. The nanomaterials are usually 10−9 m in size that means it is one billionth of a meter. The nanomaterials show different physicochemical properties than the bulk material which inherently depends on their size and shape. Surprisingly the nanomaterials produce a unique character with new characteristics and capabilities by modifying the shape and size at the nanoscale level. Nanomaterials may be of different shapes like nanorods, nanoparticles, nanosheets which can be characterized based on their dimensionality. Nanomaterials with zero-

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dimensional are nanoparticles, one dimensional is nanorods or nanotubes and two dimensional are generally films and layers type one. These are categorized mainly for the single isolated nanomaterials. By the interaction of two or more particles, their physical properties will alter. These particles of different constituents are called bulk or three-dimensional nanomaterials Based on the dimensions of nanoscale (<100 nm) they are classified as follows.

- Zero-dimensional nanomaterials (0-D): In this, all the three dimensions of the nanomaterials are in the nanoscale range. Nanoparticles will come into this classification.
- One dimensional nanomaterial (1-D): In this, in any one dimension it will be in nanoscale range and remaining two dimensions are out of the nanoscale range. Nanorods or nanotubes or nanowires are related to this class.
- Two-dimensional nanomaterials (2-D): Any two dimensions are in nanoscale range and remaining one dimension is out of it. These include nanofilms, nanolayers, and nanocoatings.
- Three dimensional or bulk nanomaterials (3-D): In any dimension, these nanomaterials are not in nanoscale range. That means in three arbitrarily dimensions they are >100 nm scale. These include nanocomposites, core shells, multi nanolayers, bundles of nanowires, bundles of nanotubes [2].

The nanomaterials are of different types based on their morphology,size, properties and the constituent in it. They are carbon-based nanomaterials, metal nanoparticles, semiconductor nanomaterials, polymeric nanomaterials, lipid-based nanomaterials.

❖ Carbon based nanomaterials:

The main constituent in this type of nanomaterials is the carbon. Carbon nanotubes and fullerenes are related to this type. Basically, the CNTs are embedded with graphene sheets which are rolled into a tube. These are much stronger than steel and can be useful for structural enhancement. The CNTs are of a single- walled type and multi-walled type. Fullerenes are the hollow cage structure particles with sixty or more carbon atoms. These are allotropes of carbon. Its structure similar to hollow football with pentagonal and hexagonal carbon units is organized in a regular pattern. They show good electricalconductivity, electron affinity, and high strength.

❖ Metal based nanomaterials :

The starting materials of the metal nanomaterials are divalent and trivalent metal ions. There are different methods for the preparation of metal nanoparticles like chemical or photochemical methods. By using reducing agents the metal ions are reduced to the metal nanoparticles. These have a high surface area and have the good adsorption ability of small molecules. They are widely used in different research areas, environmental and bioimaging studies. Not only a single nanoparticle but also the mixing of two or more nanoparticles with the size control can also be achieved. By doping different metals even the rare earth metals can change the main element characteristics. By doping different elements in different constitutions their properties also get vary

❖ Semiconductor nanomaterials

Semiconductor nanomaterials have metallic and non-metallic properties. They exhibit wide band gaps by modifying it shows different properties. These are widely used in photocatalysis, electronic devices. For instance, ZnS , ZnO , CdS , CdSe ,CdTe are related to group II-VI semiconductor materials.GaN , GaP , InP , InAs are from group III-V. Inrecent times, semiconductor grapheme nanocomposites attracted the researches. The graphene can improve the physical and chem-ical properties of the semiconductor. For gas sensing sensitivity, piezoelectric properties graphene composites materials can be utilized.

❖ Nanocomposites

The nanocomposite is a polyphase solid material where one of the phases has one, two or three dimensions of less than 100 nm. Nanocomposites have a high surface to volume ratio which differs from typical composites. Based on the size and the shape the physicochemical properties may differ as follows. There are different types of nanocomposites like that of nanomaterials. The different types are

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Ceramic Matrix Nanocomposites (CMNC), Metal Matrix Nanocomposites (MMNC) and Polymer Matrix Nano composites (PMNC).

2. Synthesis of nanomaterials

The synthesis of nanoparticles can be done by three different approaches. They are as follows. Biological methods, Physical, methods Chemical methods. The biological method is simple and easy, generally with a single step, eco-friendly. In this context, we can use the microorganisms and also the different plant parts for the preparation of the nanomaterial.

Use of bacteria:

By biomineralization process, the living organisms will participate in synthesizing the nanoparticles by using a protein. For instance, at the bottom of the sea, in anaerobic conditions magnetotactic bacteria prepare the magnetic particles as a compass to the direction of their preferred habitat by the use of magnetosomes which is a protein-coated for the synthesis of nanosized magnetic iron oxide crystals. In in vitro conditions, the core diameter of 20–45 nm homogeneous particles may be produced.

Use of Fungi:

Fusarium oxysporum fungus was used for the preparation of extracellular silver nanoparticles. These are long term stable nanoparticles due to the enzymatic activity of NADH-reductase.the higher amount of protein secretion is observed in fungal cells than the bacterial cells. Nowadays in food, animal feed, medicines, paper, and textile industry, T. reesei is widely using.

Use of algae:

Singaravelu et al. proposed the extracellular gold nanoparticles preparation from Sargassum wightii algae. Within 12 h of incubation 95% production was achieved. Research regarding the nanoparticle preparation by the use of algae is not explored more. The disadvantages of this process are some bacteria, fungi and algae are pathogenic and therefore safety measures want to build up.

Preparation of nanomaterials by using different plant parts:

The plants and plant extracts have also been used for the synthesis of the nanoparticles. The metal nanoparticles get reducedby the phytochemicals present in the plants. The phytochemicals like flavones, organic acids, quinonesare naturally acted as good reducing agents for nanoparticle preparation. The gold nanoparticles of different shapes are synthesized from the biomass of Medicago sativa (alfalfa) plant, Pelargonium graveolens (Geranium) plant leaves. Bimetallic Au, Ag, and bimetallic Au core-Ag shell nanoparticles are synthesized from Azadirachta indica(neem)leaves

3. Characterization of nanomaterials:

The nanoparticles exhibit different physicochemical properties. Onvarying their size and even a small dimension in nanoscale they will exhibit differenproperties. To examine their properties characterization of nanoparticles wants to be donewith different instruments. They are UV Spectrophotometer, Fourier Transform Infrared (FT-IRSpectroscopy, Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) Scanning Electron Microscopy (SEM), Vibrating Sample Magnetometer (VSM),

Applications of nanoparticles:

Ferrite nanoparticles are almost widely used in each and every field due to their magnetic, electrical, optical and chemical properties. Their applications range from medical to modern industries. They are applied in the area of biomedical, wastewater treatment, catalyst, information technologies. They are used as sensors and biosensors in which electrochemical, optical, piezoelectric and magnetic field are applicable. In energy storage devices they are applicable in the form.

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Future prospects:

While nanotechnology remains a dream window into the future of biomechanics and medicine for many, it is not as far-fetched as many believe. In terms of medicine, there is lots of potential for functional and consistently developing future enterprises involving drug delivery systems and cell targeting to increase their efficiency, resourcefulness, and effectiveness. For instance, NP tissue engineering may result in a fundmental breakthrough in plastic surgery by producing a novel tissue.

Conclusions:

Day to day the synthesis of novel nanomaterials are increasing. The nanomaterials with mixed compositions are also synthesizing to apply in different fields. The facile synthesis methods will produce the nanoparticles of desired size, shape and property one which can withstand the external conditions but still, they need some improvement. Nowadays wide research in going into the fields of biomedicine, electronic storage devices, and sensors but still there is a scope for the development of…

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Review on Soil and agriculture chemistry

Ustad. S. F, D. K. Borolkar, Ustad H. F, Muley D. B
Chemistry Department, PG students, Shivaji Mahavidyalaya, Udgir (MH) - 413517
Email: salehaustad@gmail.com

Abstract:

Agricultural management is a key force affecting soil processes and functions. Triggered by biophysical constructions as well as rapid structural and technological developments. New management practices are emerging with largely unknown impacts on soil processes and functions. This impedes assessments of the potential of such emerging practices for sustainable intensification, a paradigm coined to address the growing demand for food and non-food products In terms of soil management. Sustainable intensification means that soil productivity is increased while other soil productivity is increased while other soil functions and services, much as carbon storage and habitat for organisms, are simultaneously maintained or even improved. In this paper we provide an overview of research challenges to better understand how emerging soil management practices affect soil processes and functions.

1. Introduction:

One of the most vital natural resources is soil. Plants are necessary for all life, and they grow in soil to meet our daily needs. Crops are grown on soils to produce food and textiles. In addition to being crucial for agriculture, soil is also more beneficial for living things. As a part of the terrestrial ecosystem, soil serves a variety of purposes, including those required to support plant growth. Since the inception of forest management as a science, people have understood the significance of soil as a storehouse of nutrients and moisture for the growth of forage and plant species. Any areas of the earth's surface that are covered in vegetation also sustain soil. The soil's state has a significant impact on how vegetation grows and is distributed. The lithosphere (rock), atmosphere (air), hydrosphere (water), and biosphere are all dynamically interconnected through soil (living things). It is the region where creatures, rocks, and the air and water that circulate around, though, and in them interact. In addition to the physical components that make up soil, its many physical, biological, and chemical components interact actively with one another. The features of a soil determine how it performs as the base of the ecosystem. The state of the soil in a specific area and on a specific scale in relation to a set of standards that encompass healthy functioning is known as the soil's health. In order to reclaim and keep our soil's capacity to function at its peak, we must carefully manage it as an ecosystem teeming with life. The term "soil health" describes the ecological balance, functionality, and ability of a soil to sustain a productive, well-balanced ecosystem with high biodiversity above and below the surface. The lithosphere (rock), atmosphere (air), hydrosphere (water), and biosphere are all dynamically interconnected through soil (living things). It is the region where creatures, rocks, and the air and water that circulate around, though, and in them interact. In addition to the physical components that make up soil, its many physical, biological, and chemical components interact actively with one another. The features of a soil determine how it performs as the base of the ecosystem. The state of the soil in a specific area and on a specific scale in relation to a set of standards that encompass healthy functioning is known as the soil's health. In order to reclaim and keep our soil's capacity to function at its peak, we must carefully manage it as an ecosystem teeming with life. The term "soil health" describes the ecological balance, functionality, and ability of a soil to sustain a productive, well-balanced ecosystem with high biodiversity above and below the surface.

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2. Characteristics of a healthy soil:

1. Good soil Tilth: In the context of a soil's suitability for crop production, soil tilth refers to the general physical characteristics of the soil. A healthy tilth is crumbly, well-structured, dark with organic matter, free of huge, hard clods, and crumbly.
2. Sufficient depth: The depth of the soil profile that allows roots to spread out and locate water and nutrients is referred to as sufficient depth. Due to historical erosion or compaction, shallow soils are more vulnerable to harm from major weather changes, putting crops at risk for stress from pathogens, floods, or drought.
3. Good water storage and good drainage: A healthy soil contains broad, stable pores that can absorb water during a strong downpour. The medium and tiny holes, which are located between these huge pores, transport the water to be stored for later use. A healthy soil's range of pore sizes enables plants to store more water during dry spells. Long rainy periods won't stop the big pores from emptying by gravity and letting in fresh air so that soil organisms and plants can grow.
4. Sufficient supply of nutrients: For optimum plant growth and to sustain a healthy cycle of nutrients within the system, there must be a sufficient and readily available supply of nutrients. In addition to toxicity for plants and microbial communities, an abundance of nutrients can cause leaching and probable ground water pollution, high nutrient runoff, and greenhouse gas losses.
5. Small population of plant pathogens and insect pests: Plant pathogens and pests can inflict diseases and crop damage in agricultural production systems. The population of these organisms is low or is less active in a healthy soil. This might be the result of direct competition for nutrients or habitat from other soil organisms, excessive parasitism, etc. Additionally, strong plants are better able to protect themselves from various pests.
6. Large population of beneficial organisms: The functioning of the soil depends on the creatures that live there. They aid in nutrient cycling, the breakdown of organic matter, the preservation of soil structure, the biological control of plant pests, and other processes. In order to perform these tasks and support the ongoing maintenance of a healthy soil condition, a healthy soil will have a vast and diversified population of beneficial organisms.
7. Low weed pressure: The pressure from weeds is a significant barrier to agricultural productivity. For water and nutrients that are crucial for plant growth, weedsPhysico-Chemical

3. **Properties in Soil Quality**:

1) pH The pH level of the soil is the most important aspect because of how it affects all other soil parameters. As a result, pH is taken into account while analysing any type of soil. A soil is described as acidic if the pH is less than 6, normal if the pH is between 6 and 8, and alkaline if the pH is greater than 8.5.
2) Soil texture In order to categorise agricultural soils according to their physical texture, soil texture is a qualitative classification tool that is used in both the field and the lab. Different regions' soil has a different texture, which is largely determined by the size of the particles and aeration is evident. It has an impact on the soil's nutrient level as well. Electrical conductivity is an important indicator of soil texture.
3) Soil moisture the amount of water that a material, such as soil, contains is known as its water content or moisture content. One of the most crucial characteristics of soil is moisture. The soil's

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ability to absorb nutrients is mostly dependent on the moisture level of the soil, which also affects the soil's texture.

4) Soil temperature the proportion of absorbed to lost energy determines the temperature of the soil. The temperature of soil varies from - 20 to 60 °C. The most significant characteristic of the soil is its temperature since it demonstrates how it affects the chemical, physical, and biological processes involved in plant growth. Season, time of day, and regional climate all affect soil temperature.
5) Electrical conductivity another crucial characteristic of soil is electrical conductivity, which is used to assess the soil's quality. It measures the number of ions in a solution. A soil solution's electrical conductivity rises as the concentration of ions does. Electrical conductivity is a rapid, easy, and affordable way to assess the health of soils. It measures the number of ions in a solution. A soil solution's electrical conductivity rises as the concentration of ions does.
6) Nitrogen The most important element that plants may acquire from the soil is nitrogen, which also serves as a growth barrier for plants. Nitrogen makes up about 80% of the atmosphere. Nitrogen gas diffuses into the water, where blue-green algae can "fix" (convert) it to ammonia for use by the algae. Inorganic nitrogen and ammonia are other forms of nitrogen that can infiltrate lakes and streams. Since nitrogen can enter aquatic systems in a variety of ways, there is a plentiful supply of nitrogen that is readily available in these systems.
7) Phosphorous every biological cell contains the essential ingredient phosphorus. It is one of the most crucial micronutrients required for plant development. Most frequently, phosphorus limits the amount of nutrients that stay in plant nucleus and serves as an energy reserve.
8) Potassium is a crucial element for the development of the plant and plays a significant function in a variety of physiological processes in plants. It is engaged in a wide range of plant metabolism events, from the creation of plant sugars for diverse metabolic requirements in plants to the regulation of photosynthesis and the formation of lignin and cellulose, which are used to construct cellular structural components.
9) Soil organic matter It is a crucial characteristic of soil. The rate of soil erosion in accelerated by a lack of organic matter in the soil. If there is soil organic matter available, then agricultural activities can exploit this soil. Animal manures, compost, and other organic materials may be put to the soil to add organic matter.

Conclusion:

For the analysis and sustainability of soil ecosystems, maintaining or improving soil quality is a more crucial criterion Establishing a precise standard for land quality, however, is a difficult task because the functions and ensuing values provided by soil ecosystems are variable and depend on the interaction of soil physical, chemical, and biological properties as well as cognitive processes, which frequently vary significantly across spatial and temporal scales. The choice of a uniform set of particular soil characteristics as measures of soil quality can be difficult and may differ between soil systems. The analysis of the review papers led researchers to the conclusion that many metrics can be used to investigate soil quality. The majority e metrics fall inside or outside the permissible ranges.

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Nanoscience & Materials Chemistry

Pooja Kharosekar
Shivligeshwar College of Pharmacy, Almala Tq. Ausa Dist. Latur - 413512
Email: poojakharosekar22@gmail.com

Abstract:

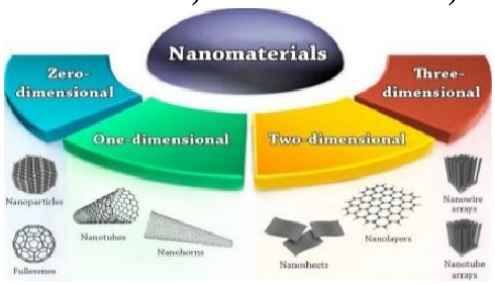
Nana science material chemistry is a multidisciplinary field that studies the properties &behavior of materials at the nanoscale or billion of materials at the combine chemistry. the impact of nanoscience emerging, the impact of nanoscience emerging science of objective that are intermediate in size between the largest molecules & smallest structure that can be fabricated by photolithograpy on future technology is discussed nanoscience contribute to almost every field of science including physics material sciencer chemistry, biology

Key Words: Nanomaterial, surface chemistry, carbon nanotubesnanoscale.

1. Introduction:

Nanoscience is the natural progression of science exploring the nature of mater between atom &molecules (defined by quantum mechanics)&condensed matter (defined by solid state chemistry (physics nanoscience is about the phenomenon that occurs in systems with nanometres dimension nanoscience is were atomics physics coverage with the physics & chemistry complex system with regard to nanoscale materials there are three general classifinactions that can used (at least for inorganics) 1) materials with delocalized electrons (insulators) materialso with new structure(usually atomically defined) materials with new structure (usually atomicalay defined) properties (or new forms of rnatter)due to their nanostructure(C60 or carbon nanotubes) Nanostrucucture can be classified according to the number of dimensions at the nanometer level.

1) Zero dimensional 2) one dimensional 3) TWO dimensional 4) Three dimensional



Flg.l.Types of nanomaterials

Materials having unique properties arising from their nanoscale dimensions Nanomaterials with fast ion transport are related also to nanoionics and nanoelectronics Nanoscalé materials can also be used for bulk applications Nanomaterials are sometimes used in solar cells which combats the cost of traditional solar silicon cells.

2. **Systems With Delocalized Electrons:** The band structures, bulk metal possesses an indefinitely extended molecular orbital. The relationship between the molecular orbital of a finite molecular system

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and the indefinite situation in a bulk metal is that the highest occupied molecular orbital CHOMO) becomes the Fermi energy Ef Of the free electron

(Fig. 1 .1). The Fermi energy depends only on the density of the electrons. If we assume that all levels up to the Ef are occupied with a total of N electrons, it can be estimated that the average level spacing is Ef/N and therefore is inversely proportional to the volume V = [43 (L = side length of particle) or O where Al wavelength of an electron with ET. The wave character of the electron is assumed here, including that the allowed values tor the wavelength A are quantized (i.e. for an electron in a box of side L, only discreet values for the energy are allowed), The properties centrally associated with bulk metals require a minimum number of electronic levels or a band. The electrons in a three-dimensional metal spread as waves of various wavelengths usually called the DE Broglie wavelength,

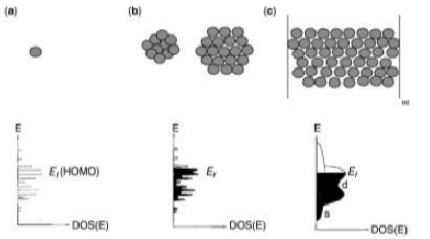
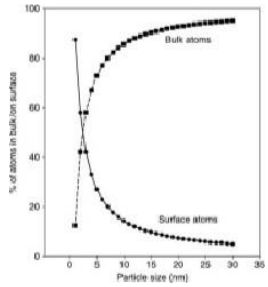


Figure 1.1 Development of the band structure of a metal: (a) molecular state, (b) nanocluster, and (c) bulk with s and d bands. (From Schmid, G. *Nanoscale Materials in Chemistry*, ed. K. J. Klabunde, New York: Wiley, 2001.)

Systems with Localized Electrons: The effects of reducing size are very different for materials with localized electrons where defects are the most significant contributor to their properties. Naturally due to the localization of electrons, the surface contains defects due to edges, corners r "f" centers, and other surface imperfections they may be thermally generated, or may arise in the course of fabrication of the solid incorporated either unintentionally or cf21iberately. Defects are important because they are much more abundant at surfaces than in E.wlk, and in nanoscale materials they become predominant due to the large surface area (Fig. 1.3). Because Of the number Of atoms at the surface and the limited number Of atoms within the lattice, the chemistry and bonding Of nanoparticles is greatly affected by the defect sites present



Applications: Nanoscience and nanotechnology are the study and application of extremely small things and can be used across all the other science fields, such as chemistry, biology, physicsr materials science, and engineering. Nanotechnology may be able to create many new materials and devices with a vast range of applications, such as in medicine, electronics , biomaterials and energy production.

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Conclusion:

Nanoscience and nanotechnology are determined by the biological concept, chemistry and material of chemistry to identify by nano mechancanism in the Nanoscience this techniques used to chemical bonds compounds and molecular formula to accurate molecular bonding some method are determined by zero dimensional measuring this all nanoscience technology Derived And Concluded The Nanoscience.

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Rational of Chromen-2-One Based Hybrid Molecules as Potential Anti-Tubercular Agents and Their Docking For Mtb.

Siddheshwar B. Lonari [1] , Anil S. Kirdant*, Suresh C. Jadhavar*
Department of Chemistry, Yogeshwari Mahavidyalay Ambajogai,Dist – Beed. Pin – 431517(M.S) India.
Email:- sidlonari24@gmail.com[1] , dr.askirdant@gmail.com* ,

Abstract

Tuberculosis (TB) remains a critical global health challenge, as identified by the World Health Organization (WHO), which names it the world's leading infectious killer. Caused by *Mycobacterium tuberculosis*, TB primarily affects the lungs, leading to symptoms such as chronic cough, weight loss, and fatigue, though it can also impact other organs, including the brain, kidneys, and spine. Transmission occurs when individuals inhale droplets containing the bacteria, allowing it to reach the alveoli after passing through the respiratory tract. Currently, the FDA-approved medications for TB treatment include rifampin, isoniazid, pyrazinamide, and ethambutol. This study aims to develop a naturally occurring compound through synthetic chemistry, targeting TB with modifications at side chains to achieve lower IC50 values compared to existing drugs. For the Synthesized of substituted amide Derivatives **(3a – 3j)** to achieve this, a library of amides was synthesized and coupled with a chromen molecule is **Compound 4a – 4 j.** the final synthesized compound was subjected to pharmacokinetic studies and molecular docking to evaluate its efficacy.

Keywords: - Tuberculosis, Anticancer, Antidiabetic activities, , Umbelliferone (7-Hydroxy 4 Methyl coumarin), Amides.

1. Introduction

For the millennia, human civilizations have relied on nature and its products as medicine, with traditional healing practices across cultures drawing on the therapeutic properties of plants, animals, fungi, and microorganisms (Fokunang CN et.al, 2011). The diverse array of natural products they produce contains biologically active compounds that have been harnessed for treating various ailments and enhancing overall health and wellness (Ekiz E et.al, 2023). Plants have been a primary source of medicinal compounds. Plant species contain chemical compounds known as phytochemicals (Altemimi et.al, 2017). More than a thousand phytochemicals have been identified to date, and they can be obtained from a variety of sources including whole grains, fruits, vegetables, nuts, and herbs. They are plant-derived chemical with bioactive properties for example quinones, flavonoids, polyphenols, tannins, terpenoids, alkaloids, polypeptides, steroids, saponins, coumarins. These phytochemicals display antibacterial, antidiarrheal, anthelmintic, antiallergic, antispasmodic, and antiviral properties as well as significant antioxidant activity (Kumar A et al, 2023). Of these phytochemicals mentioned coumarin is widespread in nature and more than 1300 coumarins have been identified as secondary metabolites from plants, bacteria, and fungi (Tsivileva et.al, 2022). Coumarin is a colorless, crystalline substance that tastes bitter and has a sweet, vanilla-like aroma. It is utilized as a flavoring agent in food products such baked goods, alcoholic beverages, and tobacco as well as in the fragrance industry (Lončar et.al, 2020). It has wide range of pharmacological properties such as anti-inflammatory, anticoagulant, antibacterial, antifungal, antiviral, anticancer, antihypertensive, antitubercular, anticonvulsant, antiadipogenic, antihyperglycemic, antioxidant, and neuroprotective properties (Venugopala et.al, 2013). 'Coumarin', the name is derived from the plant

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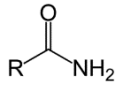
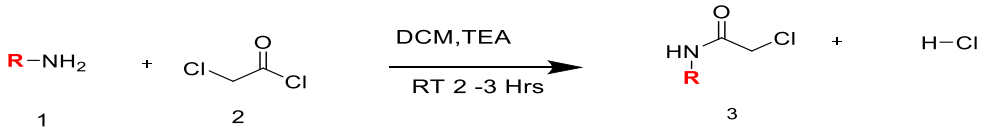
Coumarouna odorata and was isolated by Vogal in 1820 (Lončar et.al, 2020). Coumarins belong to the benzopyrone family commonly found in many medicinal plants. In this work, a total of 10 Amides are synthesized from anilines, pyridines and chloroacetyl chloride, Triethylamine and Dichloromethane (DCM).

General Reaction: - Respective Anilne to N Phenyl Acetamide Respective Aniline/pyridine is taken as starting material the reagent used is chloroacetyl chloride, Triethyl amine and the solvent used is Dichloromethane (DCM).The progress of the reaction is checked through thin layer chromatography

2. Synthesis of chloroacetamides



Amides- These are functional groups in which a carbonyl carbon atom is connected to a nitrogen atom, an H-atom, or a C-atom by a single bond.



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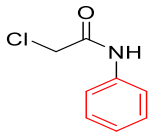

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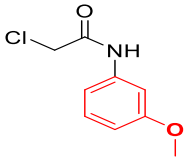

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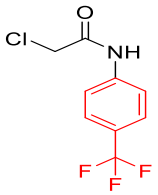

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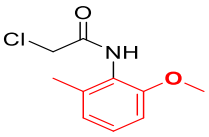

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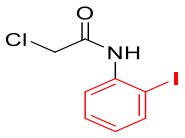

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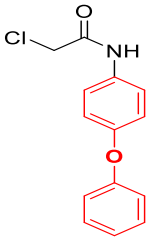

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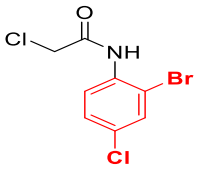

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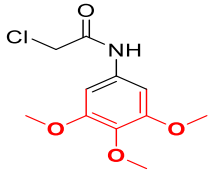
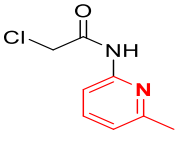
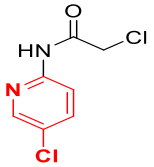


3 h



3 i



3 j

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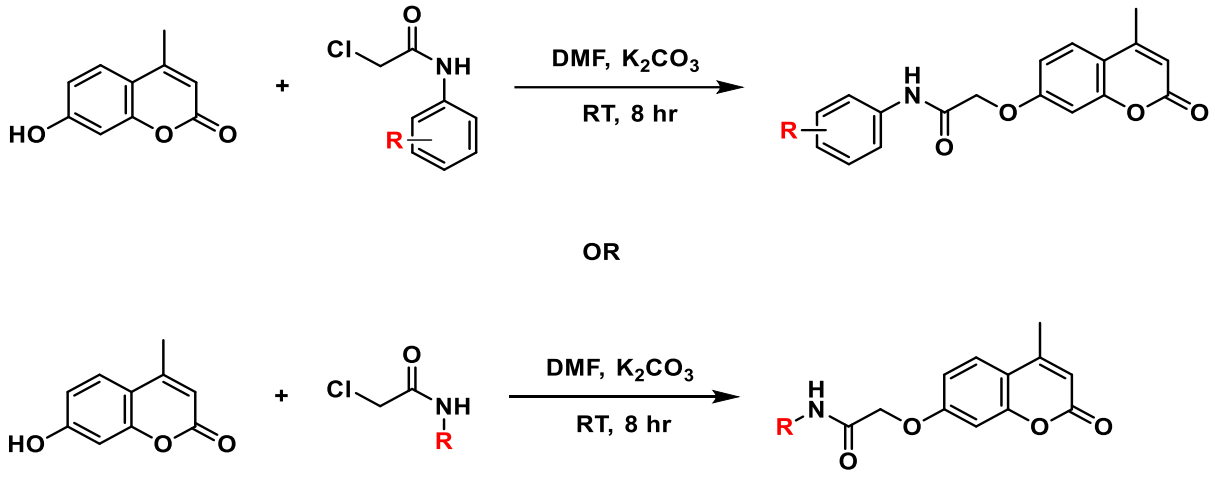
3. Materials And Methods: -

Tuberculosis (TB) is caused by bacterium Mycobacterium tuberculosis. TB affects the lungs, it can also affect other parts of the body like brain, the kidneys or the spine. TB is treated with a combination of antibiotics for a period of six to nine months or longer. The most common drugs used for TB treatment include isoniazid, rifampicin, pyrazinamide, and ethambutol. Here, our study is to find molecule which is more effective than the marketly available drugs. Chromen-2-one is a naturally occurring compound which has anticancer, anticonvulsant, antimicrobial, anticholinesterase, antituberculosis, and antidiabetic activities. Chromen-2-one is synthetically modified to produce 7-hydroxy-4-methyl-2H-chromen-2-one (7-Hydroxy-4-methyl-coumarin) to get a better antituberculosis activity. Series of amide was prepared and set of amide was coupled with 7-hydroxy-4-methy.l-2H-chromen-2-one. The objective is to check the biological activity of the coupled molecule and to know if it is a promising drug candidate. Insilico studies is to be done.

4. Synthesis Of Chromen Molecule (7-Hydroxy-4-Methyl- 2h-Chromen-2-One)

A mixture of resorcinol (1.101 g, 0.01 mole) and ethyl acetoacetate (1.274 ml, 0.01 mole) with 75% H_2SO_4 (10 ml) was heated for one hour. The resulting dark green solution was cooled and poured over crushed ice and filtered using vaccum pump. The thin-layer chromatography (TLC) was checked with reference, the reference taken is Umbelliferone (7-Hydroxy coumarin). The both compound exhibited fluorescence in UV light chamber. There was slight impurity in the compound formed, so the compound is to separate using column chromatography until clear spot is visible in the TLC plate. To identify whether the compound formed is chromen molecule the compound is sent to Mass spectroscopy and H^1 NMR. The compound structure is elucidated. The next step is to couple this pure compound formed (7-hydroxy-4-methyl-2H-chromen-2-one) with the amide which shows best activity towards Tuberculosis (TB).

5. Experimental



Coupling Of Chromen Molecule With Chloroacetamide: In coupling reactions, two similar or different species react together to yield a new product. There is a common intermediate and a metal catalyst.

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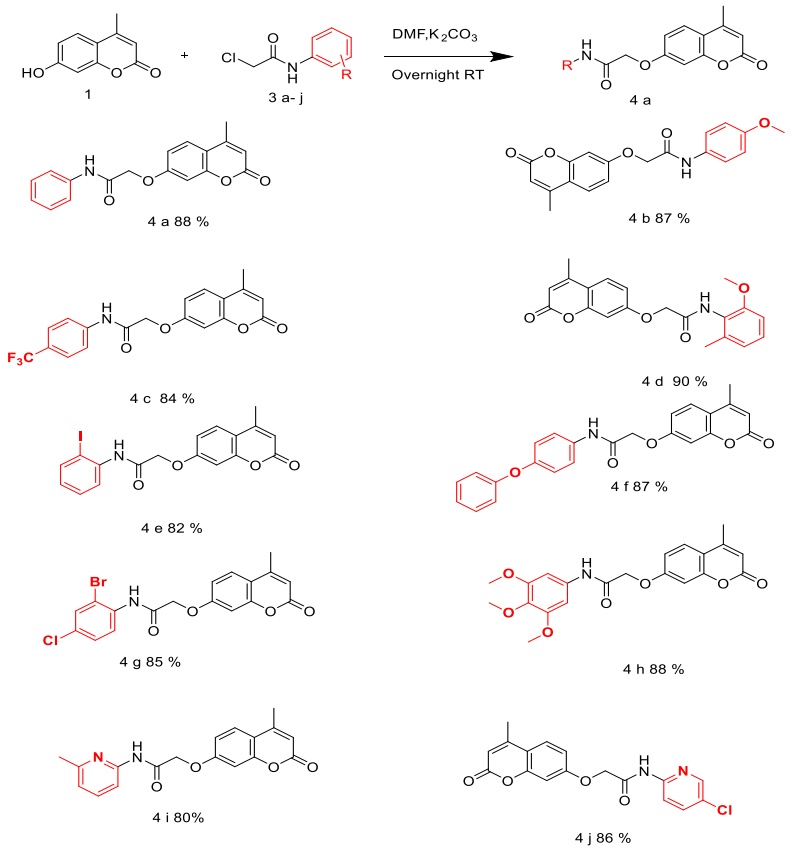
General Procedure of the synthesis of 7-hydroxy-4-methyl-2H-chromen-2-onemolecule N- Phenyl acetamide:- Here in the coupling reaction, the reactants taken are the 7-hydroxy-4-methyl-2H-chromen-2-one molecule (1eq) and the corresponding amide (1.3 eq) with K_2CO_3 as base and DMF as solvent, the reaction is done at room temperature and kept overnight.



Scheme 1- 7-hydroxy-4-methyl-2H-chromen-2-one molecule N-Phenylacetamide**.**

6. Results and Conclusion: -

The main molecule used in the reaction is Chromen-2-one molecule. A series of intermediates(amides) are made and are coupled with the Chromen molecule. Insilico studies like molecular docking is performed to determine the receptor-ligand interaction. Drug likeness is validated through pharmokinectics and ADME studies. The coupled complex should be validated for their biological activity The complex giving positive results are taken for further studies.

Molecular Docking

Here in this work, the coupled final product is taken as ligand and the receptor used is DNA Gyrase receptor.First we have to prepare protein and ligand

Preparation of protein (Receptor): Protein was downloaded from Protein Data Bank and is downloaded in PDB format. The downloaded protein is prepared using AutoDock Vina(Version 1.5.7).The heteroatoms, water

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molecules should be removed, Polar H may be added while preparing protein.We can also select grid-box in the target protein and thus prepared protein can be saved as PDBQT (Protein Data Bank, Partial Charge (Q), & Atom Type (T))format.

Preparation of Ligand: The ligands taken are the final coupled compound. The structure of the final compound is drawn by ChemBioDraw Ultra 14.0 tool and is saved is "mol" Files. These prepared ligands energy can be minimized by the OpenBabel tool in the PyRx Software and these energy minimized ligands can be saved in PDBQT Format.

Table 1: Interaction of Ligands with the receptor

PROTEIN	LIGAND	DOCKING SCORE	INTERACTING RESIDUE	INTERACTIONS
3IG0	**4 - A**	-5.7	VAL A:630, PRO A:578	Hydrogen Bond, Hydrophobic Interaction(Pi-Pi stacked, Pi alkyl)
3IG0	**4 - B**	-6.5	SER A:541, ALA A:531, LEU A:529, LEU A:563, ALA A:533, THR A:542	Hydrogen Bond(conventional hydrogen bond, carbon hydrogen bond), Hydrophobic interactions(Pi-Pi stacked, Alkyl, Pi-Alkyl)
3IG0	**4 - C**	-7.2	SER A:541, ASP A:532, ALA A:531, GLY A:537, ARG A:634, VAL A:636, ASP A: 640, LEU A:563	Hydrogen Bond(Conventional Hydrogen Bond, Pi-Donor Hydrogen Bond), Halogen(Halogen(Fluorine)), Electrostatic(Pi-anion,)
3IG0	**4 - D**	-5.4	ILE A:513, ILE A:506, LEU A:497	Hydrogen Bond(Conventional Hydrogen Bond), Electrostatic (Pi-cation), Hydrophobic(Pi-Pi stacked, Pi-alkyl)
3IG0	**4 - E**	-6.8	ARG A:550, ARG A:553, ASP A:645, HIS A:514	Hydrogen Bond(Conventional Hydrogen Bond), Electrostatic (Pi-Anion), Hydrophobic(Pi-alkyl)
3IG0	**4 - F**	**-7.5**	VAL A:630, PHE A:580, VAL A:632	Hydrogen Bond(Conventional Hydrogen Bond), Hydrophobic(Pi-alkyl, Pi-Pi T shaped, Pi-sigma)
3IG0	**4 - G**	**-7.2**		
3IG0	**4 - H**	**-6.7**	ARG A:634, ALA A:644, ALA A:563, ALA A:643, ALA A:566, ALA A:533	Hydrogen Bond(Conventional Hydrogen Bond), Electrostatic (Pi-cation), Hydrophobic(Pi-sigma, Alkyl, Pi-alkyl)
3IG0	**4 - I**	**-6.4**	SER A:541, ALA	Hydrogen Bond(Conventional

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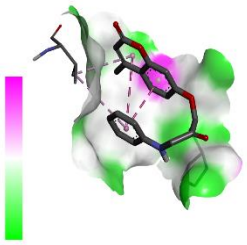
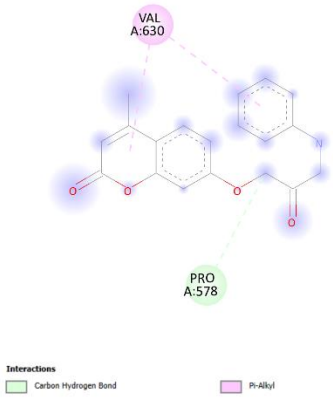
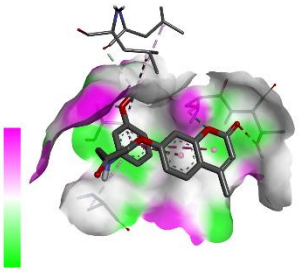
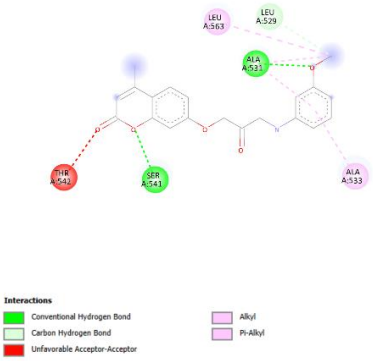
			A:644, ALA A:531, ALA A:563	Hydrogen Bond), Hydrophobic(Alkyl, Pi-Alkyl)
3IG0	**4- J**	**-5.8**	PRO A:578, THR A:624, VAL A: 630, GLU A:623	Hydrogen Bond(Conventional Hydrogen Bond), Hydrophobic(Pi-sigma, Amide-Pi stacked)

Table 2: Docking results of 10 compounds

COMPOUD	3-D INTERACTION WITH RECEPTOR	2-D INTERACTION
4 - A		
4 - B		

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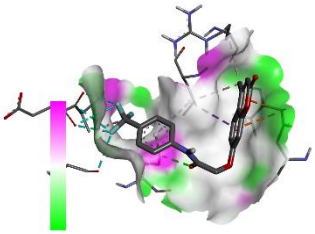
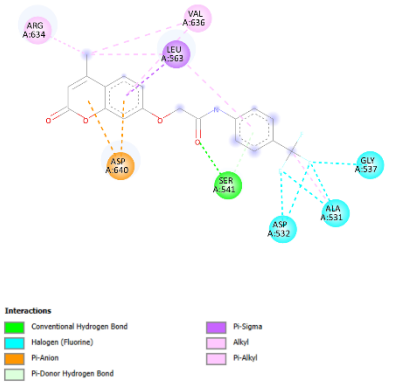
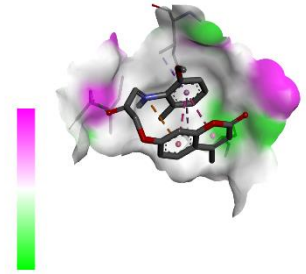
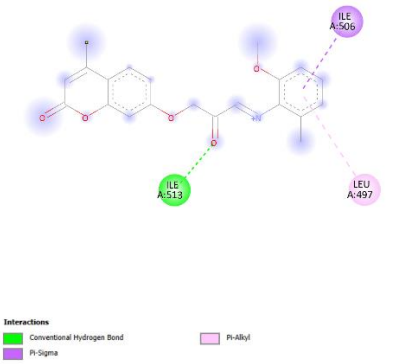
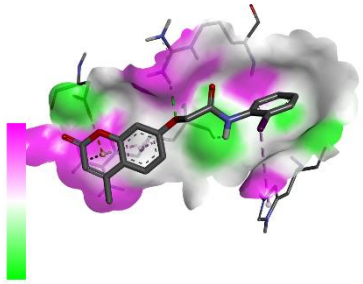
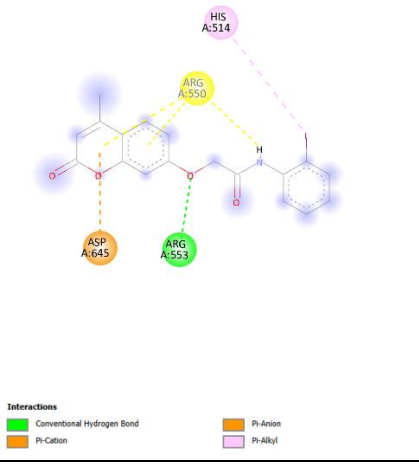
4 - C		
4 - D		
4 - E		

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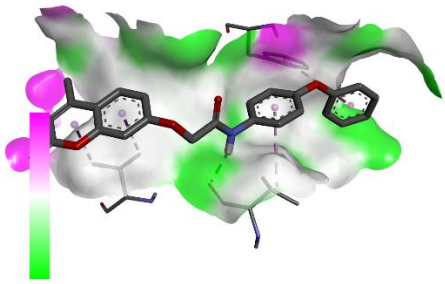
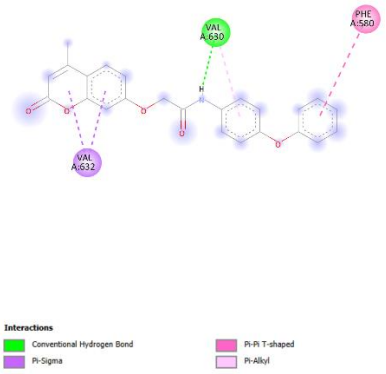
4 - F		
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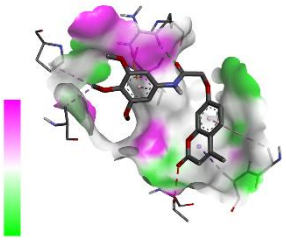
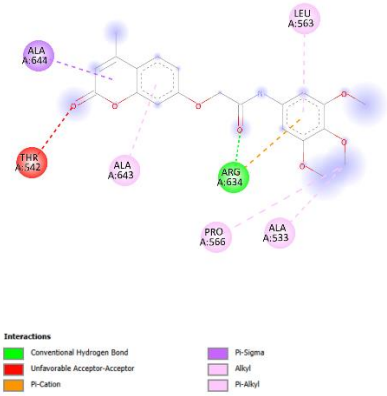
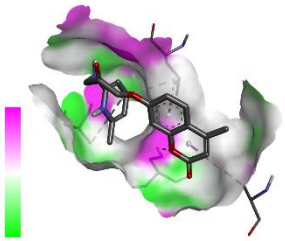
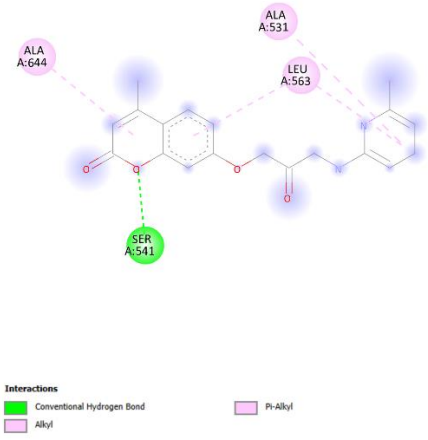
4 - H		
4 - I		

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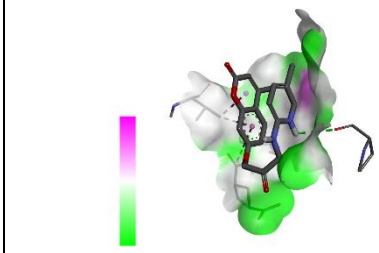
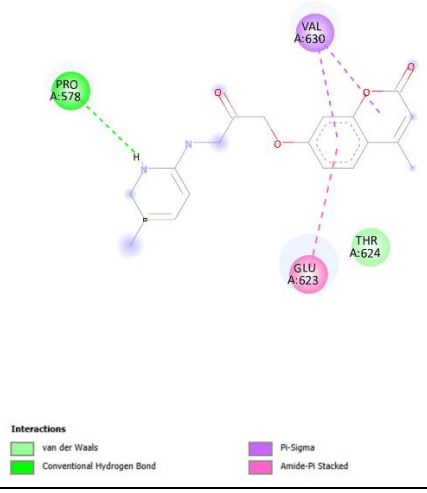
4 - J		

7. Pharmacokinetics

Pharmokinetic study is done using SWISS-ADME.It helps to compute physicochemical descriptors as well as to predict ADME parameters, pharmokinetic properties, drug-likeliness and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery. For the lead molecule to be drug-like molecule it should pass Lipinski's rule of five.

- hydrogen bond donors not greater than 5
- hydrogen bond acceptors not greater than 10
- molecular weight not greater than 500 Da
- octanol-water partitioncoefficient (logP)

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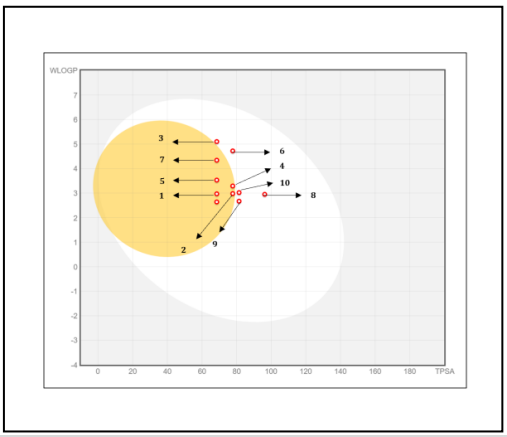
Table 3: Pharmokinetic analysis of the final compounds

	4 - A	4 - B	4 - C	4 - D	4 - E	4 - F	4 - G	4 - H	4 - I	4 - J
Mol wt.	323.34	353.37	377.31	367.4	435.21	401.41	422.66	399.4	338.36	358.78
Heavy atoms	24	26	27	27	24	30	25	29	25	25
Aromatic heavy atoms	16	16	16	16	16	22	16	16	16	16
Fraction Csp3	0.16	0.2	0.16	0.24	0.11	0.08	0.11	0.24	0.21	0.17
Rotatable bonds	6	7	6	7	5	7	5	8	6	6
H Bond acceptor	4	5	7	5	4	5	4	7	5	5
H Bond Donor	1	1	1	1	1	1	1	1	1	1
iLOGP	2.33	2.92	3.05	3.25	3.03	3.38	3.38	3.12	2.81	2.8
XLOGP3	3.69	3.66	4.01	3.59	3.35	4.66	4.02	2.61	2.92	3.15
MLOGP	1.95	1.63	2.97	1.86	2.85	2.96	3.23	1.21	1.5	1.81
Solubliliy(ESOL LogS)	-4.27	-4.33	-4.75	-4.36	-4.81	-5.35	-5.14	-3.84	-3.86	-4.13
GI Absorption	High	High	High	High	High	High	High	High	High	High
BBB Permeability	Yes	Yes	No	Yes	Yes	No	Yes	No	No	No
Log Kp	-5.65	-5.86	-5.75	-5.99	-6.58	-5.44	-6.02	-6.88	-6.29	-6.25
Lipinski violations	0	0	0	0	0	0	0	0	0	0
PAINS	0	0	0	0	0	0	0	0	0	0

8. Boiled Egg:-

The BOILED-Egg in SWISS-ADME is to predict simultaneously two key ADME parameters, i.e. the passive gastrointestinal absorption (HIA) and brain access (BBB).



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9. Experimental Data:-

^{1}H and 13 C NMR

4- a. 2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)-N-phenylacetamide (GO-PhQm):^{1}H NMR (400 MHz, DMSO) δ 10.16 (s, 1H), 7.73 (d, *J* = 8.7 Hz, 1H), 7.66 – 7.61 (m, 2H), 7.36 – 7.30 (m, 2H), 7.12 – 7.02 (m, 3H), 6.24 (t, *J* = 1.2 Hz, 1H), 4.85 (s, 2H), 2.41 (s, 3H).

^{13}C NMR (100 MHz, DMSO) δ 166.31, 161.31, 160.55, 155.00, 153.86, 138.76, 129.26, 127.05, 124.26, 120.14, 114.12, 112.87, 111.92, 102.14, 67.75, 18.61.

4-c.N-(3-methoxyphenyl)-2-((4-methyl-2-oxo-2H-chromen-7-yl) oxy) acetamide (GO-QmAm-6):

^{1}H NMR (400 MHz, DMSO) δ 10.15 (s, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.33 (t, *J* = 2.2 Hz, 1H), 7.27 – 7.17 (m, 2H), 7.08 – 7.01 (m, 2H), 6.70 – 6.64 (m, 1H), 6.24 (d, *J* = 1.5 Hz, 1H), 4.85 (s, 2H), 3.73 (s, 3H), 2.41 (s, 3H).

^{13}C NMR (100MHz, DMSO) δ 166.36, 161.30, 160.55, 159.97, 154.99, 153.87, 139.95, 130.08, 127.05, 114.11, 112.86, 112.31, 111.92, 109.67, 105.85, 102.13, 67.71, 55.48, 18.62.

4 -d.N-(2-methoxy-6-methylphenyl)-2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)acetamide (GO-QmAm-2): 1 H NMR (400 MHz, DMSO) δ 9.45 (s, 1H), 7.73 (d, J = 8.7 Hz, 1H), 7.17 (t, J = 7.9Hz, 1H), 7.10 – 7.01 (m, 2H), 6.93 – 6.87 (m, 1H), 6.83 (d, J = 7.6 Hz, 1H), 6.25 (d, J = 1.3 Hz,1H), 4.85 (s, 2H), 3.76 (s, 3H), 2.42 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, CDCl 3) δ 171.20, 166.05, 158.65, 141.90, 132.66, 131.65, 127.14, 118.00, 116.64, 114.32, 106.89, 72.38, 60.72, 23.37, 23.05.

4 e. N-(2-iodophenyl)-2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)acetamide (GO-QmAm-4) : ^{1}H NMR (400 MHz, DMSO) δ 9.64 (s, 1H), 7.91 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.67 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.14 – 7.08 (m, 2H), 7.01 (m, *J* = 7.6, 1.6 Hz, 1H), 6.25 (d, *J* = 1.4 Hz, 1H), 4.89 (s, 2H), 2.41 (d, *J* = 1.2 Hz, 3H).

^{13}C NMR (101 MHz, DMSO) δ 166.55, 160.82, 160.54, 154.99, 153.86, 139.45, 138.89, 129.40, 128.17, 127.12, 126.20, 114.34, 112.89, 112.07, 102.43, 95.88, 67.75, 18.64.

4f .2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)-N-(4-phenoxyphenyl)acetamide (GO-QmAm-9) : ^{1}H NMR (400 MHz, DMSO) δ 10.20 (s, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.40 – 7.34 (m, 2H), 7.14 – 6.95 (m, 7H), 6.24 (d, *J* = 1.4 Hz, 1H), 4.85 (s, 2H), 2.41 (s, 3H).

4g .N-(2-bromo-4-chlorophenyl)-2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)acetamide (GO-QmAm-8 : ^{1}H NMR (400 MHz, DMSO) δ 9.77 (s, 1H), 7.85 (d, *J* = 2.4 Hz, 1H), 7.76 (dd, *J* = 8.6, 6.9 Hz, 2H), 7.50 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.09 (d, *J* = 8.5 Hz, 2H), 6.26 (d, *J* = 1.4 Hz, 1H), 4.92 (s, 2H), 2.42 (s, 3H).

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4h. 2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)-N-(3,4,5-trimethoxyphenyl)acetamide (GO-QmAm-12): ^{1}H NMR (400 MHz, DMSO) δ 10.09 (s, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.08 – 7.01 (m, 4H), 6.25 (d, *J* = 1.3 Hz, 1H), 4.83 (s, 2H), 3.74 (s, 6H), 3.62 (s, 3H), 2.41 (d, *J* = 1.3 Hz, 3H).

4 i.: 2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)-N-(6-methylpyridin-2-yl)acetamide (GO-QmAm-14 :^{1}H NMR (400 MHz, DMSO) δ 10.62 (s, 1H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.75 – 7.65 (m, 2H), 7.05 – 6.97 (m, 3H), 6.24 (d, *J* = 1.3 Hz, 1H), 4.93 (s, 2H), 2.43 (s, 3H), 2.41 (s, 3H).

4j. N-(5-chloropyridin-2-yl)-2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)acetamide (GO-QmAm-17) :^{1}H NMR (400 MHz, DMSO) δ 10.88 (s, 1H), 8.42 (d, *J* = 2.6 Hz, 1H), 8.08 (d, *J* = 9.0 Hz, 1H), 7.93 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.05 – 6.99 (m, 2H), 6.24 (d, *J* = 1.2 Hz, 1H), 4.96 (s, 2H), 2.41 (s, 3H).

Author Contribution

Siddheshwar B. Lonari: Conceptualization, Experiment, Analysis, Manuscript draft preparation, editing.

Anil S. Kirdant: Conceptualization and Guidance.

Suresh C. Jadhavar: Conceptualization, formal editing, and guidance.

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A study on Chalcone Analogues-versatile with Medicinal and Biological Potential

Syeda Neha B.S.J., Tekale A.S, Reddy P.S., Muley D.B.

Chemistry Department, PG students in Shivaji Mahavidyalya Udgir, (MH)-413517

Email:nehasyeda34@gmail.com, reddypravin50@gmail.com

Abstract

This review's main focus is on the most recent synthesis of chalcones with N, O, or S heterocycles, highlighting their biological potential. Chalcone derivatives are considered in beneficial species because they possess a keto-ethylenic moiety, -CO−CH=CH−. Due to the existence of a reactive α, β-unsaturated carbonyl group, the synthesis of chalcone derivatives, which have been physiologically explored for use against specific disease targets, has been made possible by recent advances in heterocyclic chemistry. The need for novel drugs that are effective against multidrug-resistant pathogens has been driven by the growth in antibiotic resistance brought on by a variety of reasons. Chalcones are phenolic compounds that fall within the flavonoids category. They are a part of a large category of naturally occurring bioactive substances. During this review we have gone through a number of studies where chalcones were created via Claisen-Schmidt condensation of suitable acetophenone with suitable aromatic aldehydes in the presence of an aqueous solution of potassium hydroxide and ethanol at room temperature in an effort to create antibacterial agents. The synthesis of diverse chalcone derivatives was motivated by the potential activity of naturally occurring chalcones as anticancer, anti-inflammatory, antibacterial, antioxidant, and antiparasitic characteristics, as well as by their unique chemical structural structure. Flavonoids and isoflavonoids, which are frequent chemical building blocks found in a variety of naturally derived compounds, are enhanced by chalcone. This review may prove to be helpful for the creation and design of new powerful therapeutic medications.

Keywords: Chalcones analogs, Biological properties, Flavonoids, acetophenone

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1. Introduction:

Chalcone is a compound consisting of two aromatic rings linked by an unsaturated alpha, beta-ketone, with various substituents on the two aromatic rings. Chalcone can be easily found in most of plants naturally and is an intermediate precursor of flavonoids and isoflavonoids. It was reported to have a wide range of applications in the fields of biology and biochemistry such as antitumor, anti-inflammatory, and antimalarial agents. Chalcones are the natural phytoconstituents having functional groups in an aromatic ketone and an enone that forms important moiety for a variety important for biological significance, which are jointly known as chalcone. Chalcones are natural phytoconstituents widely distributed in plants that originate in the flavonoid family including chalcones, which are secondary metabolites of edible or medicinal plants. The foundation of chalcone 1, 3-diphenyl-2-propen-1-ones is two aryl moieties connected by an alpha, beta-unsaturated carbonyl group. The structure of these compounds has a -C=O-CH=CH- keto-ethylenic moiety. They have an order that contains delocalized pi electrons in their aromatic rings. Chalcones, which greatly contribute to the coloration of the corolla of various plants, are mostly composed of polyphenolic compounds with hues ranging from yellow to orange. Chalcones occur naturally in a variety of foods, including fruits, vegetables, cereals, flowers, tea, roots, stems, and wine.

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Medicinal Significance of Chalcone Analogs:

Chalcones are - unsaturated ketones containing the reactive keto-ethylenic group –CO-CH=CH-. (Figure 1). The presence of a double bond in conjugation with carbonyl functionality is believed to be responsible for the biological activities of chalcones, as the removal of this functionality makes them inactive. The conjugated double bond produces the delocalization of π electrons which reduces its electrophilic character and makes it an intermediate for the synthesis of various biologically important heterocycles such as pyrazoline, oxazoline, thiazine, oxazine, pyrimidine, etc.

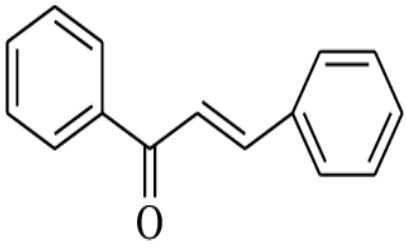

Fig: 1 Chalcone

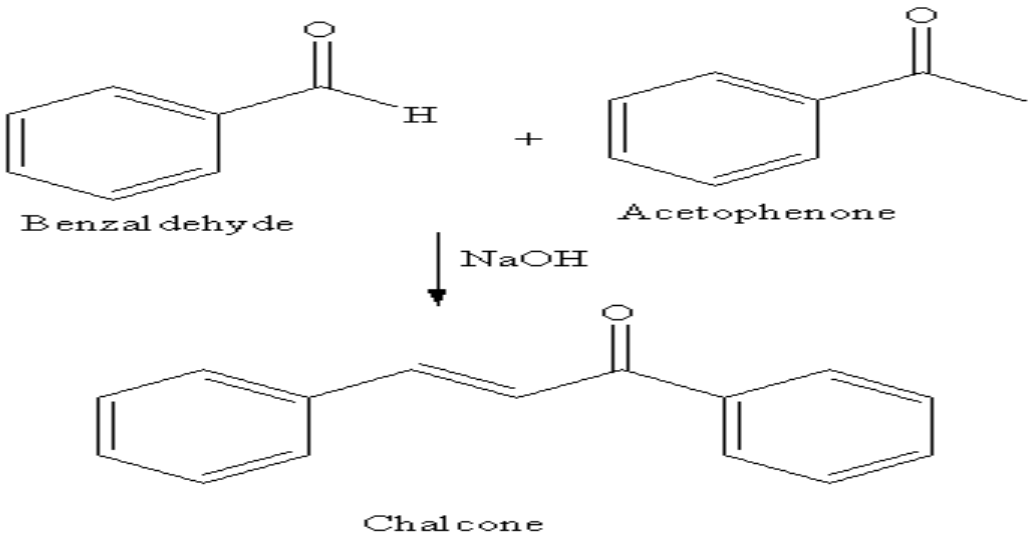

Fig: 2 Reaction of Chalcone

2. Methodology:

A number of chalcones were created via Claisen Schmidt condensation of suitable acetophenone with suitable aromatic aldehydes in the presence of an aqueous solution of potassium hydroxide and ethanol at room temperature in an effort to create antibacterial agents. IR and NMR spectrum data were used to describe the produced molecules. A series of chalcones prepared by

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Claisen Schmidt condensation of suitable acetophenone with suitable aromatic aldehydes in thepresenceof an aqueous solution of potassium hydroxide and ethanol at room temperature.

Anticancer:

A complex illness that kills millions of people every year globally, cancer is brought on by unchecked cell growth. The potential for chalcone compounds to have anticancer activity through a variety of physiological mechanisms has been studied. The developed chalcone compound with a novel anticancer-related mode of action, diverse chalcone derivatives are designed and synthesized. Variously substituted poly-methoxy chalcone components were prepared. Anticancer therapies employ a number of methods, such as surgery, chemotherapy, and radiation, either alone or in combination. Major obstacles to effective cancer therapy include side effects and multidrug resistance. Chalcones are one example of a phytochemical that has been found to be affordable, accessible, and comparatively harmless. Chalcones have the ability to target important molecular processes that may contribute to the genesis and spread of cancer.

Antimalarial

Malaria is a major parasitic infection disease in the world, caused by *Plasmodium falciparum*. Chalcones are precursors of numerous plant metabolites with distinctive scaffolds owing to exceptional biological properties. The main structure is 1, 3-diphenyl-2-propene-1-oness, the two benzene rings are associated by highly electrophilic three-carbon alpha, beta-unsaturated carbonyl configuration. Chalcone derivatives have been tested for its antimalarial activity against *P. falciparum*. Chalcone drugs are used by the treatment of malaria. The available medicines such as chloroquine is no longer effective in the treatment of malaria, due to the increasing of multiple drug resistance. *P. falciparum* and *P. vivax* are the two major human malaria parasites. The majority of deaths are caused by *P. falciparum*, which has become resistant to almost all treatments. It is understandable why chalcones' antimalarial action has attracted so much attention. A Michael addition of nucleophilic species to the double bond of the enone is likely the cause of the strong antimalarial activity of several chalcones.

Antiviral:

The chalcone derivatives mainly, nucleosides have generated widespread interest due to their antiviral properties. An example of a chalcone analog that is utilized as an antiviral. Since the dawn of time, several viral epidemics have wracked the globe. The ongoing appearance and spread of new viral illnesses have compelled researchers to look for fresh therapeutic approaches that can get beyond the drawbacks of antiviral medications that are already on the market. Chalcone are natural studies on the suppression of plant viruses and human rhinoviruses led researchers to the discovery of chalcones' antiviral capabilities. Chalcones have varying antiviral activity, which implies that the antiviral activity of each chalcone is dependent on certain patterns of substitution.

Antibacterial:

More and more research are being done on chalcones' antibacterial properties. Many research teams have either synthesized or altered naturally occurring chalcones or have isolated and characterized the structure of chalcones with antibacterial activity. The capacity of the, -unsaturated ketone to undergo a conjugated addition to a nucleophilic group, such as a thiol group in an important

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protein, has been linked to bactericidal effects. A number of a-triazolyl chalcones were created, and the created substances showed strong antibacterial and antifungal activity. In a different investigation into the antibacterial action of three chalcones, diuvaretin, uvaretin, and isouvaretin, it was shown that only gram-positive bacteria were inhibited from growing in culture.

Antifungal:

It is intriguing to note that chalcone derivatives only displayed activity against dermatophytes and no other types of fungi, as dermatophytes are a group of fungi that typically infect the keratinized areas of the body and dermatomycoses are very challenging to treat. Using the agar dilution technique, Lopez *et al.* investigated chalcones against a panel of human opportunistic pathogenic fungi. An intriguing has been published on the effect of the substituents on ring A. A number of chalcones were created in an effort to create antimicrobial agents using the Claisen-Schmidt condensation of suitable acetophenones with suitable aromatic aldehydes in the presence of an ethanol and potassium hydroxide aqueous solution at room temperature. By using their IR, 1H-NMR spectrum data, and elemental analyses, the produced substances were identified. The cup plate technique was used to evaluate each compound's antibacterial and antifungal properties. Crotmadine, a compound that displayed antifungal action, was isolated from the leaves and stems of *Crotalaria* madarosis Wight & Arn. An ethanol extract of the leaves of *Maclure tinctoria* (L.)

Anti-inflammatory:

Numerous chalcones and their derivatives have been mentioned in the literature as having potential to inhibit cyclooxygenase (COX). The results of a study using a carrageenan-induced hind paw edoema model to evaluate the anti-inflammatory effects of new chalcone derivatives revealed that the 5′-chloro-2′-hydroxy-4′6′-dimethyl-3, 4, 5-trimethoxy chalcone exhibited the most potent anti-inflammatory activity with a 90% inhibition of edoema]. Another research examined the inhibitory effects of a new family of indole-based chalcones on COX-1 and COX-2, and found that COX-1 was remarkably inhibited. The nitrogen-containing chalcone derivatives demonstrated inhibition of certain inflammatory process-related enzymes, including trypsin, COX-2, and -glucuronidase. In a different study, it was found that artificial fluoro-hydroxy substituted pyrazole chalcones had a selective inhibitory effect against the COX-2 enzyme and a moderate effect against the COX-1 enzyme. The suppression of COX-2 was related to the activity. Nitric oxide (NO) and prostaglandin E2 (PGE2) production suppression has been suggested as a possible treatment for a variety of inflammatory illnesses. Damage to tissues might result from high NO levels. It has been shown that activated macrophages produce an excessive amount of NO in inflammatory disorders like rheumatoid arthritis. Therefore, it would be intriguing to create NO inhibitors that are strong and focused for possible therapeutic applications.

Antimicrobial:

Chalcones are well-known chemical building blocks used to create a variety of heterocyclic compounds. According to reports, chalcone-based compounds contain a variety of biological properties, including antibacterial properties. Release of chemical mediators, leukotriene B4 production, tyrosinase activity, and aldose reductase activity are all inhibited. The antibacterial action of chalcones is discovered to be caused by the presence of a reactive, -unsaturated keto function. Ten fresh chalcones based on thiazoles were created and there *in-vitro* antifungal capabilities were examined as part of ongoing research into the development of novel antimicrobials. These had little antifungal efficacy against all of the investigated fungi and were less potent than ketoconazole and bifonazole. The antibacterial activity of the produced compounds was examined *in-vitro* using the agar cup-plate technique. The outcomes showed good antibacterial and antifungal activity.

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Antidiabetic:

According to reports, chalcones may have an inhibitory effect against alpha-glucosidase or alpha-amylase.

Result and conclusion:

The synthesis of diverse chalcone derivatives was motivated by the potential activity of naturally occurring chalcones as anticancer, anti-inflammatory, antibacterial, antioxidant, and antiparasitic characteristics, as well as by their unique chemical structure. Flavonoids an isoflavonoids, which are frequent chemical building blocks found in a variety of naturally occure compounds, are enhanced by chalcone Conclusions A special template called a chalcone is connected to several biological processes. The compounds or extracts of chalcone-rich plants may be used as medications or food preservatives due to the phenolic groups' radical quenching characteristics. This review article has listed the anti-infective and anti-inflammatory properties of several chalcones. The literature is analyzed to provide a meaningful overview of the structural requirements

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Sugar and Alcohols: Mannitol, Sorbitol, Xylitol and Erythritol

*Biradar Mohan Bhimrao &*Panchal Bapurao Dagdu, **Tekale A.S.,**Reddy P.S.
*Chemistry Department PG student in Shivaji Mahavidyalaya ,Udgir, MS, India
** Faculty in Chemistry Department Shivaji Mahavidyalaya,Udgir, MS, India
Email: biradarmohan548@gmail.com, reddypravin50@gmail.com

Abstract:

The sugar alcohols commonly found in foods are sorbitol, mannitol, xylitol, erythritol, isomalt, and hydrogenated starch hydrolysates. Sugar alcohols come from plant products such as fruits and berries. Sugar alcohols occur naturally and at one time, mannitol was obtained from natural sources. Today, they are often obtained by hydrogenation of sugars and other techniques. Sugar alcohols do not contribute to tooth decay. Consumption of sugar alcohols may affect blood sugar levels, although less than of sucrose. Sugar alcohols, with the exception of erythritol, may also cause bloating and diarrhea when consumed in excessive amounts. Mannitol and sorbitol are isomers, the only difference being the orientation of the hydroxyl group on carbon 2. Among production methods of mannitol are Industrial synthesis, Biosyntheses, Natural extraction, chemical process, microbial process. Most sorbitol is made from corn syrup, but it is also found in apples, pears, peaches, and prunes. It is converted to fructose by sorbitol-6-phosphate 2-dehydrogenase. Xylitol is a "tooth-friendly", nonfermentable sugar alcohol. It appears to have more dental health benefits than other polyalcohols. The structure of xylitol contains a tridentate ligand, (H-C-OH)3 that can rearrange with polyvalent cations like Ca2+. This interaction allows Ca2+ to be transported through the gut wall barrier and through. Xylitol is produced by hydrogenation of xylose, which converts the sugar (an aldehyde) into a primary alcohol. Another method of producing xylitol is through microbial processes, including fermentative and biocatalytic processes in bacteria, fungi, and yeast cells, which take advantage of the xylose-intermediate fermentations to produce high yield of xylitol. In the body, most erythritol is absorbed into the bloodstream in the small intestine, and then for the most part excreted unchanged in the urine. About 10% enters the colon. Because 90% of erythritol is absorbed before it enters the large intestine, it does not normally cause laxative effects. Chemical and fermentative processes have been introduced for largescale production of erythritol. Erythritol can be synthesized from dialdehyde starch by high-temperature chemical reaction in the presence of a nickel catalyst.

Key Words: Xylitol,Erythritol,Biofuels, Sorbitol,Mannitol,biorefinery ,thermal integration,co-products,sustainable development

1. Introduction:

Sugar alcohols (also called polyhydric alcohols, polyalcohols, alditols or glycitols) are organic compounds, typically derived from sugars, comprising a class of polyols. Contrary to what the namemay suggest, a sugar alcohol is neither a sugar nor an alcoholic beverage. They are white, water-soluble solids that can occur naturally or be produced industrially from sugars. They are used widely in the food industry as thickeners and sweeteners. In commercial foodstuffs, sugar alcohols are commonly used in place of table sugar (sucrose), often in combination with high intensity artificial sweeteners to counter the low sweetness. Xylitol is perhaps the most popular sugar alcohol due to its

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similarity to sucrose in visual appearance and sweetness. The sugar alcohols commonly found in foods are sorbitol, mannitol, xylitol, isomalt, and hydrogenated starch hydrolysates. Sugar alcohols come from plant products such as fruits and berries. The carbohydrate in these plant products is altered through a chemical process. The carbohydrate in these plant products is altered through a chemical process. These sugar substitutes provide somewhat fewer calories than table sugar (sucrose), mainly because they are not well absorbed and may even have a small laxative effect. Many so-called "dietetic" foods that are labeled "sugar free" or "no sugar added" in fact contain sugar alcohols. People with diabetes mistakenly think that foods labeled as "sugar free" or "no sugar added" will have no effect on their blood glucose. Sugar alcohols have the general formula $HOCH_2$ (CHOH) nCH2OH. In contrast, sugars have two fewer hydrogen atoms, for example $HOCH_2$ (CHOH)nCHO or $HOCH_2(CHOH)n-1C(O)CH_2OH$. The sugar alcohols differ in chain length. Most have five- or six-carbon chains, because they are derived from pentoses (five-carbon sugars) and hexoses (six-carbon sugars), respectively. They have one OH group attached to each carbon. They are further differentiated by the relative orientation (stereochemistry) of these OH groups. Unlike sugars, which tend to exist as rings, sugar alcohols do not. They can however be dehydrated to give cyclic ethers, e.g. sorbitol can be dehydrated to isosorbide. Sugar alcohols occur naturally and at one time, mannitol was obtained from natural sources. Today, they are often obtained by hydrogenation of sugars, using Raney nickel catalysts.

2. Methods:

In this cross-sectional analysis, HTGC was assessed by proton . Habitual consumption of alcoholic and nonalcoholic beverages was assessed using a validated food-frequency questionnaire. All beverages were converted to standard servings and to percentage of tot energy intake (En%). We performed linear Regression to examine the association of alcoholic and nonalcoholic beverages with HTGC, adjusted for age, smoking, education, ethnicity, physical activity, total energy intake, and total body fat. We studied replacement of alcoholic beverages with nonalcoholic beverages per 1 serving/d and per 5 En%/d.

3. Objective:

We aimed to study the consumption of alcoholic and nonalcoholic beverages and their mutual replacement in relation to hepatic triglyceride content (HTGC) in middle-aged men and women.

4. Health effects:

Sugar alcohols do not contribute to tooth decay (Bradshaw and Marsh, 1994). Consumption of sugar alcohols may affect blood sugar levels, although less than of sucrose. Sugar alcohols, with the exception of erythritol, may cause bloating and diarrhea when consumed in excessive amounts.

Common sugar alcohols:

Erythritol (4-carbon), Iditol (6-carbon), Fucitol (6-carbon), Glycerol (3-carbon), Volemitol, Threitol (4-carbon), Inositol, Arabitol (5-carbon), Isomalt (12-carbon), Xylitol (5-carbon), Maltitol (12-carbon), Ribitol (5-carbon), Mannitol (6-carbon), Sorbitol (6-carbon), Galactitol (6-carbon)

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Both disaccharides and monosaccharides can form sugar alcohols; however, sugar alcohols derived from disaccharides (e.g. maltitol and lactitol) are not entirely hydrogenated because only one aldehyde group is available for reduction. The simplest sugar alcohol, ethylene glycol, is sweet but notoriously toxic.The more complex sugar alcohols are for the most part nontoxic.

Mannitol:

Mannitol is a type of sugar which is also used as a medication (Wakai et al, 2013). As a sugar it is often used as a sweetener in diabetic food as it is poorly absorbed from the intestines. As a medication it is used to decrease high pressures in the eyes such as are seen in glaucoma and to lower increased intracranial pressure. Medically it is given by injection. Effects typically begin within 15 minutes and last up to 8 hours. Common side effects from medical use include electrolyte problems and dehydration. Other serious side effects may include worsening heart failure and kidney problems. It is unclear if use is safe in pregnancy. Mannitol is in the osmotic diuretic family of medications and works by pulling fluid from the brain and eyes. The discovery of mannitol is attributed to Joseph Louis Proust in 1806. It is on the World Health Organization's List of Essential Medicines, the most effective and safe medicines needed in a health system. The wholesale cost in the developing world is about 1.12 to 5.80 USD a dose. In the United States a course of treatment costs 25 to 50 USD. It was originally made from the flowering ash and called manna after its supposed resemblance to the Biblical food.

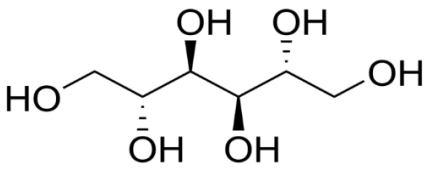

Fig:1 Manitol

Biosynthesis:

Mannitol is one of the most abundant energy and carbon storage molecules in nature, produced by a plethora of organisms, including bacteria, yeasts, fungi, algae, lichens, and many plants. Fermentation by microorganisms is an alternative to the traditional industrial synthesis. A fructose to mannitol metabolic pathway, known as the mannitol cycle in fungi, has been discovered in a type of red algae (Caloglossa leprieurii), and it is highly possible that other microorganisms employ similar such pathways.

Natural extraction:

Since mannitol is found in a wide variety of natural products, including almost all plants, it can be directly extracted from natural products, rather than chemical or biological syntheses. In fact, in China, isolation from seaweed is the most common form of mannitol production. Mannitol concentrations of plant exudates can range from 20% in seaweeds to 90% in the plane tree. It is a constituent of saw palmetto (Serenoa). Traditionally, mannitol is extracted by the Soxhlet extraction, utilizing ethanol, water, and methanol to steam and then hydrolysis of the crude material. The mannitol is then recrystallized from the extract, generally resulting in yields of about 18% of the original natural product. Another & upcoming method of extraction is by using supercritical and

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subcritical fluids. These fluids are at such a stage that there is no difference between the liquid and gas stages,and are therefore more diffusive than normal fluids. This is considered to make them much more effective mass transfer agents than normal liquids. The super-/sub-critical fluid is pumped through the natural product, and the mostly mannitol product is easily separated from the solvent and minute amount of byproduct. Enzymatic production of mannitol Mannitol can be enzymatically produced from fructose in a one pot synthesis by using NADH-dependent MDH or NADPHdependent MDH. Saha purified MDH from L. intermedius B-3693 and showed that the purified enzyme can convert fructose to mannitol completely in the presence of NADPH. The cofactor dependency of the enzyme is a major limitation. A number of strategies such as enzymatic, electrochemical, chemical and photochemical, and biological methods are available for cofactor regeneration (Chenault and Whitesides 1987). A two-enzyme system can be used for cofactor regeneration with simultaneous conversion of two substrates into two products of interest (Wichmann et al. 1981). One example is the simultaneous conversion of fructose and formate using the enzymes MDH and FDH (Parmentier et al. 2005) Synthesizing reaction: Fructose + NADH + H+ = Mannitol + NAD+ Regenerating reaction: Formic acid + NAD+ = CO2 + NADH

Synthesizing reaction: Fructose + NADH + H+ = Mannitol + NAD

Regenerating reaction: Formic acid + NAD+ = CO2 + NADH

Medical, Food and Nutrition Applications of mannitol:

Mannitol is used as a sweet-tasting bodying and texturing agent. It reduces the crystallization tendency of sugars and is used as such to increase the shelf life of foodstuffs. Crystalline mannitol exhibits a very low hygroscopicity, making it useful in products that are stable at high humidity. It is only about half as sweet as sucrose. Mannitol exhibits reduced physiological calorie value (1.6 kcalg−1) compared to sucrose (4 kcalg−1). It has a low solubility in water of only 18% (w/v) at 25 °C and 13% (w/v) at 14°C (Perry et al. 1997). In comparison, the solubility limit of sorbitol in water is about 70% (w/v) at 25°C. Mannitol is sparingly soluble in organic solvents such as ethanol and practically insoluble in ether, ketones, and hydrocarbons (Schwarz 1994). It forms orthorhombic crystals and the crystals have a melting point at 165–168 °C (Schwarz 1994). Mannitol is extensively used in chewing gum.

XYLITOL:

Xylitol is a sugar alcohol used as a sweetener. Xylitol is categorized as a polyalcohol or sugar alcohol (alditol). It has the formula CH2OH (CHOH) 3CH2OH and is an achiral isomer of pentane1, 2, 3, 4, 5-pentol. Unlike other natural or synthetic sweeteners, xylitol is actively beneficial for dental health by reducing caries (cavities) to a third in regular use and helpful to remineralization. Multiple studies utilizing electron microscopy have indicated that xylitol is effective in inducing remineralization of deeper layers of demineralized enamel. Fair evidence was found that xylitol (as chewing gum, lozenges, nasal spray, etc.) reduced the incidence of acute middle ear infection in healthy children.

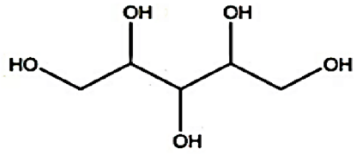

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Fig:2 Xylitol

SORBITOL:

Sorbitol, less commonly known as glucitol, is a sugar alcohol with a sweet taste which the human body metabolizes slowly. It can be obtained by reduction of glucose, changing the aldehyde group to a hydroxyl group. Most sorbitol is made from corn syrup, but it is also found in apples, pears, peaches, and prunes. It is converted to fructose by sorbitol-6-phosphate 2-dehydrogenase. Sorbitol is an isomer of mannitol, another sugar alcohol; the two differ only in the orientation of the hydroxyl group on carbon 2. While similar, the two sugar alcohols have very different sources in nature, melting points, and uses.

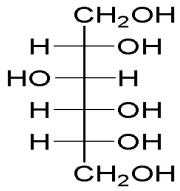

Fig: 3 Sorbitol

Conclusion:

Due to increasing epidemic of obesity and diabetes, it is important to educate consumers to make reasonable and healthy food choices. Consumption of added sugars has risen dramatically over the past few decades and has negatively contributed to human health. Foods rich in added sugar contribute mainly extra calories to diet usually without nutritional value. Unfortunately, people crave sweetness, and thus, sugar substitutes have drawn attention of consumers as well as producers and dieticians. However, human body response is not identical when we compare artificial sweeteners with those of natural origin, especially sugar alcohols that characterize with many attractive properties not only to producers but also to consumers. As these compounds are new, there is a need for education as products containing polyols are a rapidly growing category of nutraceuticals and functional food. Therefore, there is a constant need for studies regarding sugar alcohols metabolism and physiological effects on human bodies.

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A Study on Advances in organic synthesis and methodology

Shivaji Mahavidyalya Udgir, (MH)-413517
*Kote A.M., **Tekale A.S., **Reddy P.S., **Muley D.B.
*Chemistry Department, PG students in Shivaji Mahavidyalaya, Udgir
**Faculty in Chemistry Department Shivaji Mahavidyalaya, Udgir
Email: aishwaryakote7@gmail.com, reddypravin50@gmail.com

Abstract:

Organic synthesis continues to drive a broad range of research advances in chemistry and related sciences. Another clear trend in organic synthesis research is the increasing desire to target improvements in the quality of life of humankind, new materials, and product specificity. Here, a landscape view of organic synthesis research is provided by analysis of the CAS Content Collection. Three emerging research directions, enzyme catalysis, photocatalysis, and green chemistry in organic synthesis, were identified and featured based on the publication trend analysis. The realm of organic synthesis continues to witness remarkable advancements, driven by the quest for more efficient, sustainable, and versatile methodologies. This paper delves into recent breakthroughs and emerging trends in organic synthesis methods. Emphasizing the importance of sustainability and selectivity, researchers have developed novel strategies that encompass diverse transformations, catalytic systems, and reaction mechanisms. From transition-metal-catalyzed cross-coupling reactions to organocatalysis and biocatalysis, the landscape of organic synthesis has expanded significantly, offering new avenues for the construction of complex molecular architectures with high precision and atom economy. Furthermore, the integration of computational tools and automation has revolutionized reaction optimization and design, enabling rapid exploration of chemical space and accelerating the discovery of innovative synthetic routes. This paper provides an overview of key developments, challenges, and future prospects in the field of organic synthesis, highlighting the pivotal role of interdisciplinary approaches and collaborative efforts in driving scientific progress and addressing societal needs.

Keywords: Organic synthesis, advances, methodologies, sustainability, catalysis, selectivity, automation, computational tools, innovation, Green Chemistry.

1. Introduction:

Creation of organic molecules by precisely planned processes forms the framework of the synthesis discipline of organic chemistry. Organic synthesis continues to immensely impact human life and well-being, as well as its relationship with other research disciplines. Foundational knowledge from the prior two centuries of post-alchemy chemistry work has been continuing to coalesce and evolve in the 21st century through astute experimentation. Increases in the precision and efficiency in synthetic chemistry have advanced through investment in specific realms, which has resulted enhanced molecular complexity, higher synthetic yield, and greater value to other disciplines. By assessing the CAS Content Collection, herein we aim to offer a synopsis of the landscape of synthetic organic chemistry. The CAS Content Collection covers worldwide journal articles and patents, full-text substance indexing and registration, and thorough records of reaction steps and yields. It is particularly useful for quantitative analysis of global scientific publications against

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variables such as time, research area, formulation, application, and chemical composition. As a companion of this communication, a full Trend Report with thorough description and extensive data analysis is published simultaneously and available for download. By the collaboration of these author parties, it is anticipated that these communications will place the state of global research efforts in this field over the past ten years into context, offering researchers and policy makers a framework to address targets for future opportunities and applications in and related to organic synthesis.

In recent years, the field of organic synthesis has witnessed a remarkable surge in creativity and ingenuity, fueled by insights from diverse disciplines including organometallic chemistry, catalysis, biotechnology, and computational chemistry. This interdisciplinary synergy has led to the emergence of ground breaking methodologies that transcend traditional synthetic paradigms, revolutionizing the way complex molecules are assembled and manipulated. From the development of novel catalysts and reagents to the exploration of new reaction mechanisms and the integration of advanced technologies, researchers are reshaping the landscape of organic synthesis, pushing the boundaries of what is chemically achievable. This paper aims to explore the latest advances in organic synthesis methods, highlighting key breakthroughs, challenges, and opportunities that define the current state of the art. By delving into diverse areas such as transition-metal catalysis, organo catalysis, biocatalysis, and automated synthesis, we seek to elucidate the underlying principles driving innovation and showcase exemplary strategies that exemplify the transformative potential of modern synthetic chemistry. Moreover, we aim to underscore the importance of sustainability, selectivity, and scalability in the design and implementation of synthetic routes, recognizing the imperative to minimize environmental impact and maximize resource efficiency. Through a comprehensive examination of recent literature and case studies, we endeavor to provide insights into the multifaceted nature of organic synthesis, shedding light on the intricate interplay between fundamental principles and practical applications. By fostering a deeper understanding of the challenges and opportunities inherent in contemporary synthetic chemistry, we hope to inspire future generations of researchers to embark on transformative journeys that shape the future of chemical synthesis and propel scientific innovation towards new frontiers. In essence, this paper serves as a testament to the ingenuity, creativity, and collaborative spirit that characterize the vibrant landscape of organic synthesis, celebrating the diversity of approaches and the limitless potential for discovery that lie ahead. As we embark on this exploration of innovative methodologies and their transformative impact, we invite readers to join us on a journey of discovery, reflection, and inspiration, as we navigate the ever-expanding horizons of synthetic chemistry in the 20th century.

Overview of the Most Prominent Concepts and their Interconnections:

To have an overview of how concepts interact with each other in the field of organic synthesis in the recent years of 2022− 2023, the most frequently indexed concepts in journal articleswere identified and the relationships among the concepts (co.occurrences in the same document) were also determined Pairs of concepts commonly associated arevisualized based on their frequencies of co-occurrences using the VOS viewers. The synthetic concepts can begrouped into three clusters. The red cluster is composed of synthetic methods and targets, among which the most common concepts are regioselective synthesis, diastereo selective synthesis, enantio selective synthesis, green chemistry, tandem reactions, cyclization, reaction mechanisms, and C− H bond activation. A second cluster is made up of two smaller clusters (blue and green) that include concepts for the chemical and physical

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characteristics of synthetic products. Finally, a yellow cluster contains concepts relevant to human medicine. The most common pharmaceutical targets indexed are antibacterial and antitumor agents, which aim at novel therapeutics for cancers and drug-resistant bacteria during the past decades. The same analysis was performed to determine the most frequently indexed concepts in patent publications

Rising Concepts in The Field Of Organic Synthesis In The Past 22 Years:

To identify current research topics of interests, related concepts from journal publications in organic synthesis over the last 22 years were assessed. Briefly, concepts were identified when they were indexed more than 400 times in 2024 and have increased more than 50 times from 2000 to 2024. Four classes of organic substances, namely, fused heterocyclic compounds, metal−organic frameworks, ionic liquids, and triazoles, are the frequently indexed classes of organic compounds with the fastest growing rate. The four organic reaction types experiencing the fastest growth are regioselective synthesis, C−H activation, three-component reaction, and click chemistry. Regioselective synthesis appears to be growing the fastest, which may be due to its association with diastereoselective synthesis, heterocyclic compound formation, and C−H bond formation.

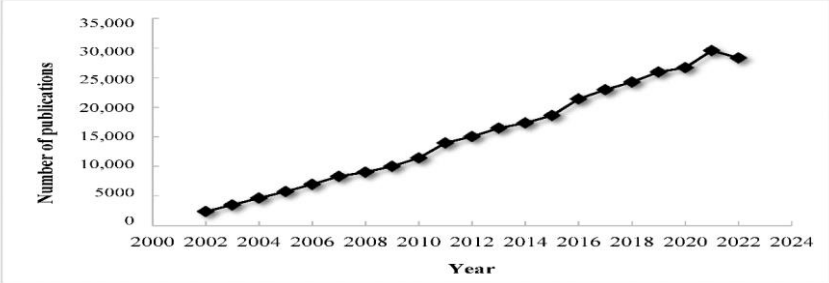

Fig:1 Rising concepts in the field of organic synthesis in the past 22 years

Recent progress in regioselective synthesis mainly focused on regioselective construction of heterocycles. The direct formation of a C−C bond from C−H bonds, instead of using a presynthesized functional group, has the potential to significantly reduce the synthetic steps and thus increase the efficiency of chemical production. The term “click chemistry”was first introduced by K. B. Sharpless in 2001 to describe reactions that are high yielding, wide in scope, stereospecific, and simple to perform in easily removable or benign solvents, which with bioorthogonal chemistry was just awarded the Nobel Prize in Chemistry in 2022. Molecular docking is a computational tool for modeling the binding of small molecules to biologically relevant components such as proteins and nucleic acids. Molecular docking informs drug design by providing chemists with the models of the relative positions of proteins and ligands, the interactions between them, and the free energies of binding. This information allows chemists to understand how changes in ligand structure affect binding and provide useful hypotheses to guide further ligand modifications for drug design. Our analysis indicates that increases in selectivity and efficiency and reduction in environmental costs are important motivations for research into organic synthesis. In particular, the development of solvents with reduced environmental costs and of methods to functionalize unactivated positions in organic substances are important research topics. The concept and publication trends we have identified

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depend on our analysis of data from the CAS Content Collection, and the popularity of a research topic inpublications may be affected not only by its scientific value and utility, but also on its economic value, the ease of research, and by stochastic variation in publication frequency. The journal trends of functional materials related concepts in organic synthesis are grouped into five categories green chemistry (including green chemistry, recycling,and biomass); drug developing (including neoplasm, pharmacokinetics, fluorescence imaging, and enzyme inhibitors) organic electroluminescent (including LUMO, and photoluminescence); property (including electric current−potential relationship, X-ray photoelectron spectra, and pore size distribution); and catalysts (including photocatalysts and
Electrochemical reduction catalysts).

Emerging Topics: Enzyme Catalysis, Photocatalysis, And Green Chemistry

Emerging research topics in organic synthesis were identifiedby evaluating clusters of newly appeared subject-concept indexes and associated documents in the CAS organic synthesis content corpus. Three topics, namely, enzyme catalysis, photocatalysis, and green chemistry, showed the most consistent and recent (in the last 10 years) publication growth in organic synthesis.

Enzyme Catalysis:

To study the global trends of research on enzymic catalysis, the number of journal and patent publications were summarized biennially to minimize the effect of variance between years. The global output of journal and patent publications shows that as a relative new research area, journal publications are the majority output on enzymic catalysis. The volume of global journal publications on this topic increasedfrom 1400 in 2011−2012 to over 1800 in 2019−2020, which isaround 30% growth over the past ten years. In contrast, patentapplications in this area are still few. The increase from 2011 to2016 was fast (around 50% increase); however, the rate of increase slowed down from 2017 to 2020 (around 15%increase). The ratio between patent and journal publications in enzyme catalysis increased from 1:7 in 2011−2012 to 1:5 in 2019−2020. Although growing, this relatively low amount of patent applications perhaps reflects a situation that many cutting-edge research discoveries have not led to practical applications yet. Four major clusters, namely, biomimetic synthesis related terms, nanoparticle- and polymer-related concepts, temperature effect related concepts, and enzyme/protein structure related concepts, can be identified from the network diagram showing the relationship between concepts indexed in enzyme catalysis-related journal documents. The heavy connections between concepts among the four clusters indicate that research in this field usually involves four aspects: reactions, reaction optimization, enzyme structure or reaction mechanism, and reaction output.

Photocatalysis:

Journal and patent publications over two-year segments in photocatalysis between 2011 and 2020 were compared. Journal publications have increased at an accelerated rate over this period, whereas patents have increased moderately compare with journals. The development of emerging concepts in photocatalysis is depicted in Figure 3. There are 1017 photocatalysis-related concepts first indexed by the CAS Content Collection in 2012−2014. C−C bond formation, tandem reaction,

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photochemical hydrogenation, and Meerwein reactions are the most indexed reaction types. Aromatic alcohols, secondary amines, and sulfoxides are the top indexed substances classes. Photoluminescence, photostability, charge separation, and the, energy-dispersive X-ray spectra are property related concepts indexed by the CAS Content Collection. In addition to half of these concepts, 1513 new relevant concepts were indexed in 2015−2017. Photosensitizers, heterogeneous catalysts, radical cyclization catalysts, and sulfonylation catalysts are the most widely used catalysts in photocatalysis. Reaction types expanded to three-component reaction, photooxidative coupling reaction, and sulfonylation. New substances involved in photocatalysis in this period are arylboronic acids, styrene, and fluoroborates. Core−shell materials and pollution related topics, such as photochemical corrosion, and environmental pollutants, are also explored. In 2018−2020, 1699 new concepts were indexed. Hydrogen evolution reaction and water splitting kinetics are hot and new concepts in this area, which may result from interest in clean energy. Hydrogen is considered as an alternative energy source to replace gasoline,and its preparation from water was studied extensively. Catalysts for three-component reaction, photocyclization, and dearomatization are new catalyst types investigated in this period.

Green chemistry:

Green chemistry is a set of methods designed to reduce environmental costs and ensure the sustainability of chemical methods. The 12 principles of green chemistry devised by Anastas and Warner constitute a summary and aspiration for chemical methods.

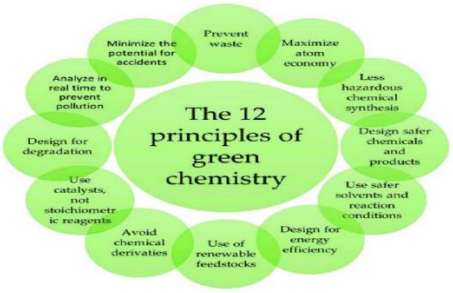

Fig:2 The 12 principles of green chemistry

Reducing the complexity of processes and their costs in reagents and solvents are some ways to achieve the goals of green chemistry. Replacing stoichiometric reagents with catalysts and replacing reductants or oxidants with electricity or light are some other ways to implement green chemistry principles. The ability to address climate change also requires more efficient chemical processes, which justifies interest in its research. The distribution of journal and patent publications on green chemistry among different countries/regions is shown in. China is leading in both journal publications and patents in this research field. Almost equal numbers of journal papers and patents were published from China over the ten year period from 2011 to 2020. India ranked second in journal publications on green chemistry followed by Iran, United
States, and Japan. In contrast, patent applications on green chemistry from countries/regions other than China are rare, which may relate to China's efforts on promoting green industries. South Korea, India, United States, and Japan are countries that contributed some patent publications in green chemistry during the past decade. The low patent activity for green chemistry indicates that few

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methods have been translated into commercialized technologies, which is consistent with a recent study on the green chemistry patent landscape.

Objective:

1. To survey and analyze recent advancements in organic synthesis methodologies across diverse areas including transition-metal catalysis, organocatalysis, biocatalysis, and automated synthesis.
2. To identify key trends, challenges, and opportunities shaping the landscape of contemporary organic synthesis, with a focus on sustainability, selectivity, and scalability.
3. To elucidate the underlying principles driving innovation in organic synthesis, including the development of novel catalysts, reaction mechanisms, and synthetic strategies.
4. To explore the integration of computational tools and automation in the design, optimization, and execution of organic synthesis reactions, highlighting their role in accelerating discovery and enhancing efficiency.
5. To showcase exemplary case studies and exemplify the practical applications of advanced synthetic methodologies in the construction of complex molecular architectures, functional materials, and bioactive compounds.
6. To critically evaluate the impact of recent advancements in organic synthesis on various scientific disciplines and industries, including pharmaceuticals, materials science, agrochemicals, and fine chemicals.
7. To foster interdisciplinary dialogue and collaboration among researchers from diverse backgrounds, recognizing the synergistic potential of cross-cutting approaches in driving scientific innovation and addressing societal challenges.
8. To inspire future research directions and stimulate curiosity-driven inquiry in the field of organic synthesis, by highlighting emerging opportunities and unexplored frontiers for discovery and exploration.
9. To contribute to the broader scientific discourse on sustainable chemistry, innovation, and technological advancement, by synthesizing and disseminating knowledge that advances our understanding of the principles and practice of organic synthesis in the 21st century.
10. To engage with and empower a diverse audience of scientists, educators, students, and industry professionals, by providing accessible insights, critical analysis, and thought-provoking perspectives on the ever-evolving field of organic synthesis.

Literature Review:

Organic synthesis has long been a cornerstone of modern chemistry, enabling the construction of complex molecules essential to a myriad of scientific disciplines and industrial applications. Over the years, the field has witnessed a remarkable evolution, driven by a relentless pursuit of more efficient, sustainable, and versatile synthetic methodologies. In this literature review, we delve into key developments and seminal contributions that have shaped the landscape of organic synthesis, highlighting notable advancements, emerging trends, and critical insights that define the current state of the art. Transition-metal catalysis stands out as one of the most transformative developments in contemporary organic synthesis. The pioneering work of pioneers such as Richard F. Heck, Ei-ichi Negishi, and Akira Suzuki has revolutionized the construction of carbon-carbon and carbon-heteroatom bonds, laying the foundation for a plethora of cross-coupling reactions that have become indispensable tools in the synthetic chemist's arsenal. From the venerable Suzuki-Miyaura reaction to the innovative Buchwald-Hartwig amination and Sonogashira coupling, transition-metal catalysis has democratized access to diverse structural motifs and enabled the streamlined synthesis of complex

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molecules with unprecedented efficiency and selectivity. In parallel, the emergence of organocatalysis as a powerful synthetic paradigm has expanded the synthetic toolbox, offering complementary strategies for the stereoselective construction of challenging molecular architectures. Catalytic enantioselective transformations mediated by small organic molecules have enabled the realization of highly efficient and atom-economical synthetic routes, facilitating access to enantioenriched building blocks and bioactive compounds with exquisite levels of stereocontrol. Notable examples include the asymmetric aldol reaction, proline-catalyzed Michael addition, and Jacobsen epoxidation, which have become hallmark reactions in the repertoire of modern synthetic chemists. Biocatalysis represents another frontier in organic synthesis, harnessing the catalytic prowess of enzymes to orchestrate complex chemical transformations under mild, environmentally benign conditions. From lipases and proteases to oxidoreductases and lyases, biocatalysts offer unparalleled substrate specificity, regioselectivity, and stereoselectivity, making them indispensable tools for the synthesis of chiral intermediates, pharmaceuticals, and natural products. Recent advances in enzyme engineering, substrate promiscuity, and biotransformation cascades have expanded the scope and versatility of biocatalysis, opening new avenues for the sustainable production of high-value chemicals and pharmaceuticals. Moreover, the integration of computational methods and automation has emerged as a game-changer in organic synthesis, accelerating reaction discovery, optimization, and scale-up. Molecular modeling, machine learning, and high-throughput experimentation have empowered researchers to explore vast chemical space, predict reaction outcomes, and design tailor-made catalysts with unprecedented precision and efficiency. Automated synthesis platforms equipped with robotic arms, reaction vessels, and analytical tools have revolutionized the way chemical reactions are conducted, enabling the rapid synthesis of diverse compound libraries and the implementation of complex synthetic sequences with minimal human intervention.

2. Methodology:

The methodology employed in this research paper integrates a multifaceted approach to investigate and advance the state of the art in organic synthesis methods. It encompasses a series of systematic and interconnected steps designed to explore novel strategies, optimize reaction conditions, and evaluate the practical applicability of synthetic methodologies. The methodology is organized into several key stages outlined below:

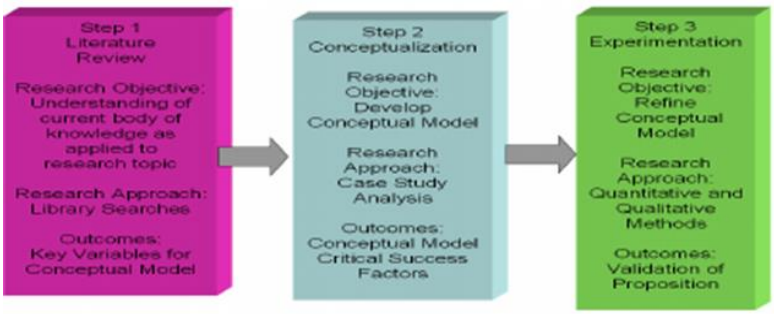

Fig: The methodology is organized into several key stages.

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Literature Review

Conduct an extensive review of the existing literature to identify recent advancements, emerging trends, and critical insights in organic synthesis methodologies. Analyze peer-reviewed articles, patents, conference proceedings, and textbooks to gather comprehensive information on key concepts, principles, and experimental techniques. Synthesize knowledge from diverse areas including transition-metal catalysis, organocatalysis, biocatalysis, computational chemistry, and automation to establish a foundation for further investigation.

Hypothesis Formulation

Formulate hypotheses based on gaps, challenges, and opportunities identified through the literature review. Define research questions and objectives to guide experimental design and data interpretation. Develop hypotheses that address specific aspects of organic synthesis, such as catalyst design, reaction optimization, substrate scope, and sustainability.

Experimental Design

Design experimental protocols and procedures to test hypotheses and validate proposed synthetic methodologies. Select appropriate starting materials, catalysts, reagents, and solvents based on their compatibility, availability, and environmental impact. Consider factors such as reaction temperature, pressure, time, stoichiometry, and analytical techniques for monitoring reaction progress and product characterization. Incorporate controls and replicate experiments to ensure reproducibility and reliability of results.

Synthetic Chemistry

Perform synthetic reactions and transformations according to the designed experimental protocols. Employ standard laboratory techniques for handling, purification, and analysis of reaction mixtures and products. Optimize reaction conditions through systematic variation of parameters and evaluation of reaction outcomes. Characterize synthesized compounds using spectroscopic, chromatographic, and crystallographic methods to confirm their identity, purity, and stereo chemical properties.

Applications:

The research paper on advances in organic synthesis methods holds significant relevance across various scientific disciplines and industrial sectors. Some of the key applications include:

Pharmaceutical Industry: Organic synthesis methods play a pivotal role in drug discovery and development by enabling the efficient synthesis of pharmaceutical intermediates and bioactive compounds. The ability to access diverse molecular architectures with high selectivity and efficiency facilitates the exploration of new drug candidates and the optimization of lead compounds for improved pharmacological properties. Materials Science: Organic synthesis methodologies are instrumental in the design and fabrication of functional materials with tailored properties and functionalities. From conducting polymers and molecular electronics to photovoltaic materials and biomaterials, organic synthesis enables the synthesis of advanced materials for applications ranging from electronics and energy storage to biomedicine and environmental remediation.

Agrochemicals and Fine Chemicals: The synthesis of agrochemicals, including pesticides, herbicides, and fungicides, relies heavily on organic synthesis methods to access structurally diverse molecules with potent biological activity. Moreover, fine chemicals such as flavors, fragrances, and

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specialty chemicals are synthesized using advanced synthetic strategies to meet stringent quality standards and consumer preferences.

Benefits Efficiency: Advances in organic synthesis methods enable the rapid and efficient synthesis of complex molecules, reducing synthetic steps, reaction times, and resource consumption. Streamlined synthetic routes facilitate the scale-up production of target compounds and enhance overall process efficiency.

Selectivity: Modern organic synthesis methodologies offer unprecedented levels of selectivity, enabling the precise control of reaction outcomes and the stereoselective synthesis of chiral molecules. Selective transformations minimize the formation of undesired by-products andenable the synthesis of complex molecular architectures with high stereochemical purity.

Drawbacks Complexity: Some advanced organic synthesis methods require specialized equipment, expertise, and resources, making them inaccessible to researchers and practitioners with limited experience or infrastructure. Complex reaction mechanisms and substrate interactions may also pose challenges in reaction design and optimization.

Cost: The implementation of certain organic synthesis methods, particularly those involving expensive catalysts, reagents, or starting materials, may incur high production costs and limit commercial viability. Cost-effective alternatives and process optimization strategies are essential to enhance the economic feasibility of synthetic routes.

Result and Analysis:

The investigation into advances in organic synthesis methods has yielded valuable insights and significant contributions to the field. The results obtained from various experiments, computational simulations, and literature analyses have provided a comprehensive understanding of the capabilities, limitations, and potential applications of modern synthetic strategies. Here, we present a summary of the key findings and their implications for the advancement of organic synthesis

Conclusion and Future Scope:

In conclusion, the exploration of advances in organic synthesis methods represents a dynamic and multifaceted journey that has unveiled new horizons of scientific inquiry and technological innovation. Through a comprehensive review of literature, experimental investigations, and computational modeling, this research paper has elucidated key principles, methodologies, and applications that define the forefront of organic synthesis in the 21st century. The synthesis of complex molecules, the discovery of novel reaction mechanisms, and the development of sustainable synthetic routes have emerged as central themes in the quest to address societal needs and propel scientific progress. The results presented in this study underscore the transformative potential of modern synthetic strategies, including transition-metal catalysis, organocatalysis, biocatalysis, and computational chemistry, in enabling the efficient and selective construction of diverse molecular architectures. From pharmaceuticals and materials science to agrochemicals and fine chemicals, the

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applications of advanced organic synthesis methods extend across diverse domains, offering solutions to pressing challenges and opening new avenues for discovery and innovation.

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Drug Design and Development

Dipmala K. Borolkar, Ustad Saleha
Department Of Chemistry, Shivaji Mahavidyalaya Udgir, (MH)- 413517

Abstract:

The Processes used by academic and industrial scientists to discover new drugs have recently experinced a true renaissance, with many new and exciting techniques being devleoped over the past 5-10 years alone. Drug design and discovery ,and research for new safe and will tolrated compounds,as well as the ineffectiveness of existing therapies , and societys insufficient Knowledge cocerning the prophylactics and pharmacotherapy of the most common diseases today , comprise a serious Challenge . This can influence not only the quality of human life, but also the health of whole societist , which became evident during Covid-19 pandemic. In general ,the process of drug development consists of three main stages : drug discovery ,preclinical development using cell-based and animal models/tests ,clinical trials on human and,finally forward moving toward the step of obtaining regulatory approval ,in order to market the potential drug.

1. Introduction:

Drug discovery is the process through which potential new medicines are identified. It involves a wide range of scientific disciplines, including biology, chemistry, and pharmacology 1-2 . In the fields of medicine, biotechnology and pharmacology, drug discovery is the process by which new candidate medications are discovered. Historically, drugs were discovered by identifying the active ingredient from traditional remedies or serendipitous discovery, as with penicillin. The development of new drugs is very complex, costly, and risky. Its success is highly dependent on intensity. Collaboration and interaction between many departments within the drug development organization, external investigators, and service providers, in constant dialogue with regulatory authorities, payers, academic experts, clinicians, and patient organizations. Within the different phases of the drug life cycle, drug development is by far the most crucial part for the initial 4-5.

Periods in Drug Discovery in Development Process:

It is roughly estimated that it takes around 5-10 years for the complete drug discovery and development process and for its introduction into the commercial market, and its costs around $1.7 Billion for the complete process to proceed successfully 6-9. The various periods/phases in the Drug discovery and development process are 10-14

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Objectives of Drug Discovery & Development:

Investigational Drug Success: Discovery/Screening: 5000-10,000, Enter Preclinical Testing: 250, Enter Clinical Testing: 5, Approved by Regulatory Bodies: 1

Drug Discovery Period: Initiate a drug discovery program, combinatorial chemistry, Lead compound series identification

Additional compounds are made: NCE‟ s identified, Drug Development & Registration Period 18, IND plan established & initiated IND filed, Clinical studies initiated, NDA prepared & submitted, Drug launched into the market

Drug Marketing & Line Expansion: Post-Marketing surveillance initiated, New clinical indications pursued,

- New dosage forms and formulations developed
- Activities conducted to support marketing and the continued success of a drug on the market

The process:

Many years, many failures, much uncertainty Most often, the development of a new medicine starts when basic scientists learn of a biological target (e.g., a receptor, enzyme, protein, gene, etc.) that is involved in a biological process thought to be dysfunctional in patients with a disease such as Alzheimer's disease (AD). Here, we are considering the discovery and development of entirely new medicines, those with a mode of action different from already approved medicines and intended for a clinical indication that is not addressed by approved medicines. Better medicines that are iterative improvements on current medications are valuable as they may offer benefits over existing medications in terms of potency, safety, tolerability, or convenience, but they usually do not involve the manipulation of biological targets different from those directly affected by existing medications. Analyses across all therapeutic areas indicate that the development of a new medicine, from target identification through approval for marketing, takes over 12 years and often much longer . The cost to develop a New Molecular Entity (NME; a small molecule compound) or New Biological Entity (NBE; an antibody, protein, gene therapy, or other biological medicine) is certainly over $1 billion and, on average, has been estimated to be about $2.6 billion , adapted from Paul et al. , shows a schematic of the stages involved in developing a new medicine along with average times required for each stage and the approximate cost (in 2010 dollars) for each phase of development.

Stages of Drug Discovery and Development Include: Target identification, Target validation, lead identification, lead optimization, Product characterization 28, Formulation and development, Preclinical research, Investigational New Drug, Clinical trials, New Drug Application 29

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Step1 Target identification and validation

Kicks off the whole drug discovery process. Naturally occurring cellular or modular structures that appear to play an important role in pathogenicity or disease progression are normally targets for therapeutics. A good target needs to be efficacious, safe and be

Target Identification and Validation:

Accessible by the drug molecule/meet clinical needs of the prospective patient. Following identification of the drug target, a systematic validation approach should be adhered to for the mode of action of lead candidate to be assessed for efficacy. The approach itself depends on the therapeutic area, but has a set of general principles that include disease association, preclinical evidence in key cells, preclinical evidence in intact systems (i.e. transgenic animals), and literature survey and competitor information 30-34.

Step 2 Hit Identification and Validation:

The obvious next step is to identify whether the small molecule leads have the desired effect against the identified targets. There are a number of approaches by which hits can be identified, *including* high-throughput screening, knowledge based approaches, and virtual screening. After initial screening, validation of hits is required, and again there are a few options to choose from

Step 3 Lead Optimization:

At this stage, the aim is to maintain the desired properties of lead compounds while improving on possible deficiencies of their structures to produce a preclinical drug candidate. This stage can be used to find out whether your drug metabolizes in the right area of the body or whether there are currently any side effects that are cause for concern. For this process, an integrated approach is recommended. The combination of specialists in computational chemistry, medical chemistry, drug metabolism, and other areas can provide unique insights into this late stage of the process.

Step 4 Late Lead Optimization:

Before progression to preclinical and clinical trials, late stage optimization, in which further pharmacological safety of a lead compound is assessed, is a vital step. If this stage is overlooked, problems in efficacy, pharmacokinetics, and safety are more likely to occur later in drug development. Safety optimization is a core stage; the aims are to identify and progress the leads with the best overall safety profile, remove the most toxic leads, and establish a well-characterized hazard and translational risk profile to enable further in vitro tests.

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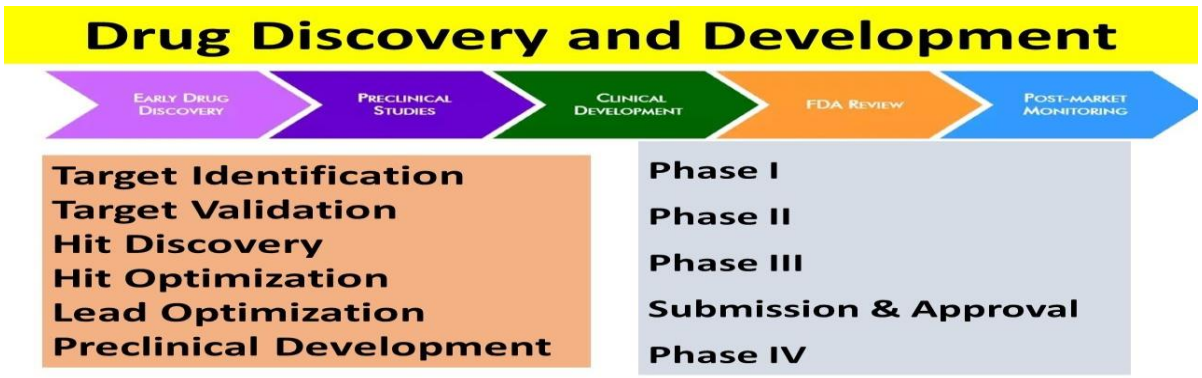

COVID-19 drug development is the research process to develop preventative therapeutic prescription drugs that would alleviate the severity of coronavirus disease 2019 (COVID-19). From early 2020 through 2021, several hundred drug companies, biotechnology firms, university research groups, and health organizations were developing therapeutic candidates for COVID-19 disease in various stages of preclinical or clinical research (506 total candidates in April 2021), with 419 potential COVID-19 drugs in clinical trials, as of April 2021.[1]

As early as March 2020, the World Health Organization (WHO),[2] European Medicines Agency (EMA),[3] US Food and Drug Administration (FDA),[4] and the Chinese government and drug manufacturers[5][6] were coordinating with academic and industry researchers to speed development of vaccines, antiviral drugs, and post-infection therapies.[7][8][9][10] The International Clinical Trials Registry Platform of the WHO recorded 536 clinical studies to develop post-infection therapies for COVID-19 infections,[11][12] with numerous established antiviral compounds for treating other infections under clinical research to be repurposed.[7][13][14][15]

In March 2020, the WHO initiated the "SOLIDARITY Trial" in 10 countries, enrolling thousands of people infected with COVID-19 to assess treatment effects of four existing antiviral compounds with the most promise of efficacy.[2][16] A dynamic, systematic review was established in April 2020 to track the progress of registered clinical trials for COVID-19 vaccine and therapeutic drug candidates.[12]

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We thank Stephane Auvin, Epileptologist and Child Neurologist, Head of the Pediatric Neurology Department, Robert Debré Hospital, for interesting discussions about the use of fenfluramine for the treatment of some forms of epilepsy.

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Effect of Synthesized Copper (II) and Silver (I) Metal Complexes with Cefuroxime on Some Cephalosporin Resistance Bacteria

N.A. Kedar,
Department of Chemistry, Dayanand Science College, Latur, Maharashtra-413512

Abstract

This study explores the development of copper (II) and silver (I) complexes with cefuroxime, a cephalosporin antibiotic, using a solvent-free mechano chemical technique. The synthesized complexes were characterized by various methods, and their structures were proposed to be [Cu (CFU) 2H2O] and [Ag (CFU) NO3], where CFU represents cefuroxime. The antimicrobial activity of these complexes against various bacterial strains, including both methicillin-resistant *Staphylococcus aureus* (MRSA) and other common pathogens, was evaluated using the disc diffusion method. The results revealed enhanced activity compared to the free ligand, suggesting potential for overcoming antibiotic resistance. Infrared spectroscopy indicated coordination of cefuroxime to the metal centers through carbonyl and carboxylate groups, along with the involvement of a water molecule in the copper complex. The distinct melting points, colors, and electronic spectra of the complexes further confirmed complex formation. This abstract effectively summarizes the key aspects of the study, including the synthesis method, complex characterization, enhanced antimicrobial activity, and proposed coordination mode. It highlights the potential of these complexes for addressing antibiotic resistance.

Keywords: Antibioticresistance, Cephalosporin, Silver, Copper.

1. Introduction

The emergence and spread of antibiotic-resistant bacteria pose a significant and growing threat to global health. Despite the development of numerous antibiotics, the constant evolution of resistance mechanisms in pathogens necessitates the ongoing search for novel antimicrobial agents. Cephalosporins, a class of β-lactam antibiotics, are crucial in combating bacterial infections, but their effectiveness is compromised by the emergence of resistant strains, particularly among species like Citrobacter freundii, Enterobacter cloacae, and Escherichia coli.

The development of new antibiotics is a complex and challenging process. The need for novel therapeutic approaches that circumvent existing resistance mechanisms is urgent. In this context, metal-based compounds have garnered considerable attention due to their diverse antimicrobial properties. Silver and copper, with their long-standing history of antimicrobial use, offer promising starting points for the development of new antibacterial agents.

Mechano chemistry, a burgeoning field in synthetic chemistry, provides an attractive alternative to traditional solution-based methods. This approach leverages mechanical energy to drive chemical reactions, often with reduced solvent usage or even solvent-free conditions, thus offering potential advantages in terms of sustainability and efficiency.Building upon our previous research on antibiotic resistance, this study investigates the antimicrobial activity of copper (II) and silver (I) complexes with cefuroxime, a second-generation cephalosporin. These complexes were synthesized mechano chemically, offering a novel approach to the development of potential antimicrobial agents

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against cephalosporin-resistant bacteria.

This introduction effectively highlights the critical issue of antibiotic resistance, emphasizes the need for new therapeutic strategies, and introduces the rationale for exploring metal-based complexes, particularly those synthesized using mechano chemical methods.

2. Materials and Methods

All the chemicals used were of analytical AR grade. The ligand used is cefuroxime (Cfu), while the metals used are copper chloride dihydrate [$CuCl_2.2H_2O$] and silver nitrate [$AgNO_3$]. IR spectra of the complexes in KBr pellets were obtained in the range of 4000-400 cm^{-1} using FTIR spectrometer. Metal analysis was determined by atomic absorption spectroscopy using perkin-Elmer Spectrometer, model 3110. UV-Vis spectra were obtained on UV-2550 Shimazu Spectrophotometer in the wavelength range of 200-800 nm.

3. Synthesis of the Complexes

Literature procedure [9] was modified and used for the synthesis of all the metal complexes by mechanochemical method. Cefuroxime (10 mmol, 4.25 g) and copper chloride dihydrate (10 mmol, 1.705 g) were weighed carefully and transferred into a mortar. The two reactants were thencrushed (ground) for twenty (20) minutes to obtain homogenous powder. The powder was removed from the mortar and stored in a desiccator. Same procedure was used for silver nitrate (10 mmol, 1.699 g) and cefuroxime (10mmol, 4.25g).

Antimicrobial Screening

The *in-vitro* antimicrobial activities of the antibiotics and their metal complexes were assayed using disc diffusion method against the following microorganisms; *Streptococcus pneumoniae, Bacillus subtillu, Salmonella typhi, Klebsielia pnuemoniae, Escherichia coli,* Methicillin- resistance *staphylococcus aureus (MRSA), Pseudomonas aeruginosa and Staphlylococcus aureus.* The suspension of each micro-organism was added to a sterile nutrient agar medium, then spread on the sterile Petri dish plates and allowed to set. Different concentrations (30, 20 and 10) mg/mLofantibioticsandtheirmetalcomplexesin methanolwereplacedonthe culturemediaandincubated for 24hrs at 37°C. Activities were determined by measuring the diameter of the zone of inhibition (mm). The antibiotics and their complexes that showed zone of inhibition of 10mmandabovewerefurtherassayedforminimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) using samples concentration of (6,4and 2) mg/mL in methanol using same bacterial species in peptone water [10].

4. Results and Discussions

The complexes of copper and silver ions obtained are air stable light green and white powders respectively. Both complexesaresolubleinpolarsolventssuchasdistilled water, methanol, ethanol and dimethylsulfoxide (DMSO). The solubility of the complexes in polar solvents, suggestthat the compounds are probably polar. Similar observation was made by [11]. The melting point of the complexes of copper and silver are 110 and 120^0C respectively (Table 1). The variation in the melting point of ligand and that of the complexes suggest formation of new compound and also evidence of complexation [12]. The molar conductivity ofthecomplexesfallsbetween3.6and4.5Scm^2/mol(Table 1). This suggest the complexes are non-

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electrolytes [13].

Infra-red spectra

The infra-red spectra data of the complexes and its ligand arepresentedinTable2.Thebandassignmentsarebased on comparison with similar studies on mixed ligand complexes and some drug based metal complexes [11]. The vibrations centered around 3190 cm^{-1}in the free ligand was assigned to v (O-H) stretching frequency, which upon complexation undergo shift in the complexes. The band at 3560 cm^{-1} in the free ligand was also assigned to v ($N-H_2$) vibration of amine group. While, the band at 1550 $cm^{-1}$was assigned to v(C=N) vibration. Similar observation was made by some workers [14].

The strong intensity band attributed to v(C=O) vibration stretching was observed in the spectra of the free ligand at 1720 cm^{-1}. The relevant bands were observed in the metal complexes with lower wavelength shift as compared to the ligand couple reduction in their intensities (Table 2). The appearance of new bands at 620 and 630 cm^{-1}in the spectraof the complexes which is assignable to v(M-O) stretching, suggest formation of the complexes.

Electronic spectra

The electronic spectral data of the cefuroxime and its complexes are presented in Table 3. Based on previous assignments of related complexes [15-17]. The transition around 349 nm in the spectra of cefuroxime (CFU) was assigned to $\pi \rightarrow \pi^*$ transition (Table 3).Similar observation was made in previous literature [17]. [Cu (CFU) 2H2O] complex showed low intensity band at 340nm assigned to MLCT. The [Ag(CFU)NO_3] complex, showed absorption band at (287, 301 and 313) nm which indicate abathochromic shift relative to the free ligand and a weak interaction between the ligand and silver ion which can be assigned to MLCT [16].

Microanalysis

The microanalytical data presented in Table 4 for the metal complexes showed good agreement with the proposed formulas, [Cu(L)2H2O] and [Ag(L)NO3], where L represents cefuroxime (CFU). This supports the proposed stoichiometry of the synthesized complexes.

Anti-microbial studies

Transition metal complexes have shown significant potential in antimicrobial and anticancer therapies [15, 18]. Previous research has explored the antimicrobial properties of Cu (I) and Ag(I) complexes [16]. Building upon these findings, this study investigated the antimicrobial activity of newly synthesized Cu (II) and Ag (I) complexes with cefuroxime, prepared using a mechanochemical approach. The antimicrobial efficacy of both the ligand (cefuroxime) and its metal complexes was evaluated against a panel of Gram-positive and Gram-negative bacteria, including *Streptococcus pneumoniae*, *Bacillus subtilis*, *Salmonella typhi*, *Klebsiella pneumoniae*, *Escherichia coli*, *Methicillin-resistant Staphylococcus aureus* (MRSA), *Pseudomonas aeruginosa*, and *Staphylococcus aureus*. [1]The results of the inhibition zone studies are summarized in Table

5. The results obtained revealed that the complexes were more effective against the microorganism than the ligand. The data also showed that Bacillus subtillus was inhibited to the greatest degree by the prepared complexes followed by Staphlyococcus aureus. While, Escherichia coli and Pseudomonas

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aeruginosa were not inhibited by both the ligand and the complexes at 10 mg/mL (Table 5). The complexes also inhibit Klebsielia pnuemoniae at concentration of 20 and 30 mg/ mL when compared with the ligand which shows less activity at same concentration.

Structure of the complexes

The analytical data of this study revealed that coordination of cefuroxime to the metal ions occurs through oxygen atom of the carboxylate anion, oxygen atom of water molecule and oxygen atom of carbonyl for both complexesto give a coordination number of five. (Fig 1 and 2). This is similar to our previous report [8]

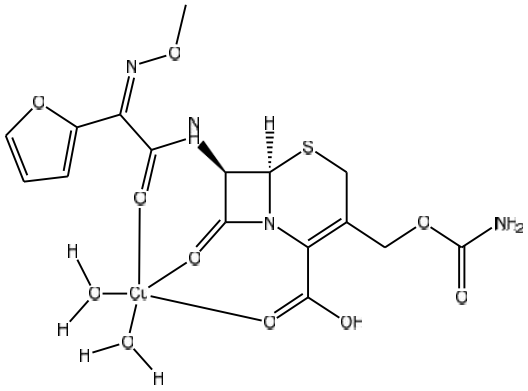

Figure1: Copper complex of cefuroxime

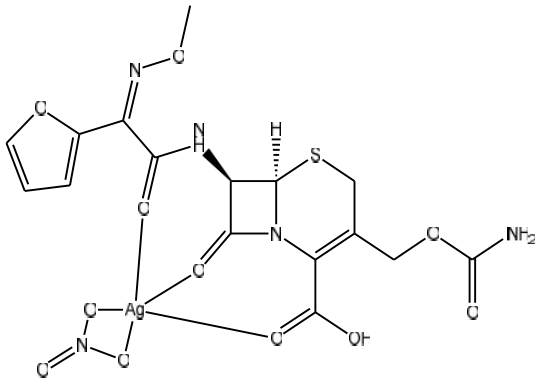

Figure 2: Silver complex of cefuroxime

Table1: Analytical data of cefuroxime and its complexes

Compounds	Molecularformula (Molarmass)	Color	Yield(g) (%)	M.pt(^{0}C)	Conductivity (Scm^2/mol)	TLC(RF Values)
CFU	$C_{16}H_{16}N_4O_8S$ (424.39)	White	-	218	-	0.5
[Cu(CFU)2H_2O]	[Cu($C_{16}H_{20}N_4O_{10}S$] (523.89)	Light green	5.61 (94.0)	120	4.7	0.9
[Ag(CFU)NO_3]	[Cu($C_{16}H_{16}N_5O_{11}S$] (594.76)	White	5.82 (98.0)	110	3.8	0.7

CFU=Cefuroxime

Table2: Infra-red spectral data of cefuroxime and its metal complexes

Compounds	v(O-H) (cm^{-1})	v(N-H) (cm^{-1})	v(C=O) (cm^{-1})	v(NH_2) (cm^{-1})	v(C=N) (cm^{-1})	v(C-S) (cm^{-1})	v(C=C) (cm^{-1})	v(M-O) (cm^{-1})
CFU	3190	1872	1720	3560	1550	2050	1235	-
[Cu(CFU)2H_2O]	3235	1890	1700	3451	1500	2030	1245	620
[Ag(CFU)NO_3]	3120	1865	1680	3473	1570	2040	1250	630

Table3: UV-V is spectra of cefuroxime and its metal complexes

Ligand/Complexes	Formula	Wavelength(nm)	Energies(cm^1)	Assignment

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CFU	$C_{16}H_{16}N_4O_8S$	350	2865	π→π*
[Cu(CFU)2H_2O]	[Cu($C_{16}H_{20}N_4O_{10}S$]	340	2941	MLCT
[Ag(CFU)NO_3]	[Cu($C_{16}H_{16}N_5O_{11}S$]	287	3484	n→π*

Table4: Micro analysis of Cu (II) and Ag (I) complexes

Compounds	**Molecularformula (Molarmass)**	**Microanalysis:found(calculated)%**			
		C	**H**	**N**	**M**
[Cu(CFU)2H_2O]	[$CuC_{16}H_{20}N_4O_{10}S$] (523.89)	36.62 (36.65)	3.80 (3.82)	10.62 (10.69)	12.15 (12.12)
[Ag(CFU)NO_3]	[$AgC_{16}H_{16}N_5O_{11}S$] (594.76)	32.01 (32.28)	2.50 (2.69)	11.75 (11.77)	18.17 (18.14)

Table5: Anti-microbial activities of cefuroxime and its metal complexes

Compounds	**Conc. mg/mL**	***MRSA***	***S.aureus***	***S.pneumoniae***	***B.subtilis***	***E.coli***	***S.typhi***	**K.*pneumoniae***	***p.aeruginosa***
CFU	10	7.0±0.8	10±0.5	0.0±0.0	12±0.5	0.0±0.0	10±0.4	0.0±0.0	0.0±0.0
	20	11±0.2	11±0.6	0.0±0.0	14±0.3	0.0±0.0	13±0.6	0.0±0.0	0.0±0.0
	30	14±0.5	13±0.4	0.0±0.0	18±0.6	0.0±0.0	16±1.0	0.0±0.0	0.0±0.0
[Cu(CFU)2 H_2O]	10	9.0±0.8	11±0.3	0.0±0.0	13±0.4	0.0±0.0	11±0.5	0.0±0.0	0.0±0.0
	20	11±0.7	14±0.8	0.0±0.0	16±0.3	0.0±0.0	16±0.4	8.0±0.0	0.0±0.0
	30	15±0.4	17±0.8	0.0±0.0	23±1.0	0.0±0.0	22±0.3	11±0.0	0.0±0.0
[Ag (CFU)NO_3]	10	9.0±0.1	11±0.2	0.0±0.0	13±0.0	0.0±0.0	8.0±0.3	0.0±0.0	0.0±0.0
	20	11±0.9	14±0.1	0.0±0.0	17±0.5	0.0±0.0	12±0.3	8.0±0.7	7.0±0.4
	30	15±0.2	17±1.0	0.0±0.0	23±0.4	0.0±0.0	15±0.5	11±0.6	9.0±0.4

MRSA= Methicillin-resistance *staphylococcus aureus, s.aureus = staphylococcus aureus, s.pneumoniae = Strepto coccus pneumonia, B.subtilis=Bacillus subtilis, E.coli= Escherichia coli, S.typhi= Salmonella typhi, K.pneumoniae=Klebsiella pneumonia and P.aruginosa= Psuedomonas aeruginosa.*

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Table6: Minimum inhibitory concentration (MIC) of cefuroxime and its metal complexes

Compounds	Conc. mg/mL	*MRSA*	*S.aureus*	*B.subtilis*	*S.typhi*	K.*pneumoniae*	*p.aeruginosa*	*E.coli*	*S.pneumoniae*
CFU	1	R	R	R	R	NA	NA	NA	NA
	2	R	R	R	R	NA	NA	NA	NA
	4	R	R	R	R	NA	NA	NA	NA
	6	R	S	S	S	NA	NA	NA	NA
	8	S	S	S	S	NA	NA	NA	NA
	10	S	S	S	S	NA	NA	NA	NA
[Cu(CFU)2H_2O]	1	R	R	R	R	NA	NA	NA	NA
	2	R	R	R	R	NA	NA	NA	NA
	4	R	R	R	R	NA	NA	NA	NA
	6	R	S	S	R	NA	NA	NA	NA
	8	S	S	S	S	NA	NA	NA	NA
	10	S	S	S	S	NA	NA	NA	NA
[Ag(CFU)NO_3]	1	R	R	R	R	NA	R	R	R
	2	R	S	R	R	NA	R	R	R
	4	R	S	S	R	NA	R	R	S
	6	R	S	S	S	NA	S	S	S
	8	R	S	S	S	NA	S	S	S
	10	S	S	S	S	NA	S	S	S

R=resistant,S=susceptibleandNA=notapplicable

From the result of minimum inhibitory concentration (MIC), it appears that both the ligand and the complexes have MIC of 6and8mg/mL on*MRSA, s. aureus, B. subtilis*and*S. typhi.* .

Table7: Minimum Bactericidal concentration (MBC) of cefuroxime and its metal complexes

Compounds	Conc. mg/mL	*MRSA*	*S.aureus*	*B.subtilis*	*S.typhi*	K.*pneumoniae*	*p.aeruginosa*	*E.coli*	*S.pneumoniae*
CFU	2	R	R	R	R	NA	NA	NA	NA
	4	R	R	R	R	NA	NA	NA	NA
	6	R	S	S	S	NA	NA	NA	NA
	8	S	S	S	S	NA	NA	NA	NA
	10	S	S	S	S	NA	NA	NA	NA
[Cu(CFU) 2H_2O]	2	R	R	NA	R	NA	NA	NA	NA
	4	R	R	NA	R	NA	NA	NA	NA
	6	R	S	NA	R	NA	NA	NA	NA
	8	S	S	NA	R	NA	NA	NA	NA
	10	S	S	NA	S	NA	NA	NA	NA
[Ag(CFU)N O_3]	2	R	R	R	R	R	R	R	R
	4	R	R	R	R	R	R	R	R
	6	R	S	R	R	R	R	R	S
	8	R	S	S	S	R	R	S	S
	10	S	S	S	S	S	S	S	S

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The MBC result also shows that both the ligand and the complexes have MBC ranging from 6-10 mg/mL on microorganism tested (Table 7).

Conclusion

The analysis of both compounds led to the proposal of five coordinated complexes. Subsequent evaluation of inhibition zones revealed that these synthesized complexes exhibited significantly enhanced antibacterial activity against cephalosporin-resistant bacteria compared to the ligand alone. This suggests that the coordination process has successfully modified the ligand's properties, resulting in improved antimicrobial efficacy.

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Green synthesis of functionalized 2, 3, 7, 8-tetrahydro-4H, 6H-pyrano [3,2g] chromene-4, 6-diones using TSIL [SBMIM] Cl^- Dr.Motegaonkar

Manorama B. Motegaonkar
[1]Department of chemistry Azad Mahavidyalaya, Ausa.
Email id: **manoramamotegaonkar42@gmail.com**

Abstract:

A fast, highly efficient and green protocol for the synthesis offunctionalized2,3,7,8-tetrahydro-4H,6H-pyrano [3,2-g]chromene-4,6-dionesat room temperature has been investigated using task-specific acidic ionic liquid (TSIL), 1-(4- sulfobutyl)-3 methy limidazolium chloride [SBMIM]Cl^-, as catalyst and green reaction medium. The reactions precede with excellent yields in short reaction times. The TSIL can be recycled for subsequent reactions with consistent activity.

Keywords: chalcones, flavanones, Kabbe condensation, Task specific basic ionic liquid [SBMIM] Cl^-

1. Introduction:

The chromanone skeleton is present in a wide variety of natural and synthetic compounds that have diverse biological and medicinal activities[1-2].In this viewpoint and persistent interest in the chemistry of advantage the chromanone motiy,[3] we endeavored to design and synthesis some novel derivatives of natural products based on the chromanone moiety for various biological applications. Chalcones and flavanones, initially isolated from natural sources are an interesting class of naturally occurring bioactive compounds with a 1,3-diarylpropane skeleton[4]. Chalcones are useful molecular scaffolds in nature and the laboratory, displaying several valuable biological activities, such as anticancer[5], anti-inflammatory[6,] and antimalerial[7] properties. It is known that chalcones are starting compounds in the synthesis of various flavonoids by means of cyclization under various conditions[8]. Flavonoids, a class of plant secondary metabolites, are built around a phenyl benzopyronestructure[9]. According to their different skeletons, they are classified into flavones, flavanones, chalcones, flavonols, isoflavones, aurones,[10] etc. The acid-catalyzed cyclization can be carried out by refluxing the chalcone in acetic acid or, alternatively, in ethanol or other suitable solvent in the presence of an acid catalyst, such as H_3PO_4[11].Anano silica-supported dual acidic ionic liquid was easily synthesized andUsed as an efficient catalyst for the synthesis of a series of new or knownflavanones[12]. These results encouraged us to further explore the spiro-chromanone– chalcone and spiro chromanone–flavanone hybrid motifs as an active pharmacophores to be exploite for further diversification and screened for antimicrobial activities.

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Herein, we describe the synthesis of novel spirochromanone-derived 2'- hydroxyl chalcones, further cyclized into flavanone derivatives, and in vitro screening results for antibacterial and antifungal activities of both series of the synthesized compounds. However, conversion of chalcones into flavanones as a rule does not proceed to completion and gives a mixture of products requiring tedious and time- consuming column chromatographic separations.15 Therefore, the objective of the present work was to develop a new method for the synthesis of flavanones by using an inexpensive, safe, and eco-friendly TSIL catalyst [SBMIM]Cl^-.

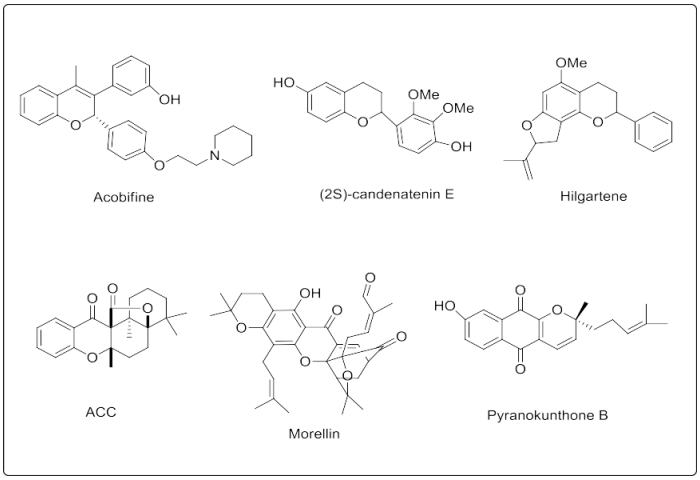

Fig. Some biologically active chromenes

2. Experimental:

1H NMR spectra were recorded in $CDCl_3$ solution at ambient temperature on a spectrometer operating at 300 MHz. Chemical shift were recorded as δ values in parts per million (ppm), and the signals were reported as s (singlet), d (doublet), t (triplet), m(multiplet) and coupling constants *J* were given in Hz. IR spectra were recorded on a FT-IR spectrometer. IR spectra of solid products were recorded in KBr and thin plates for liquid products. The purity of the compounds was tested routinely by TLC (eluent hexane–AcOEt, 4:1) on silica gel coated glass slide (Merck, Silica gel G for TLC).

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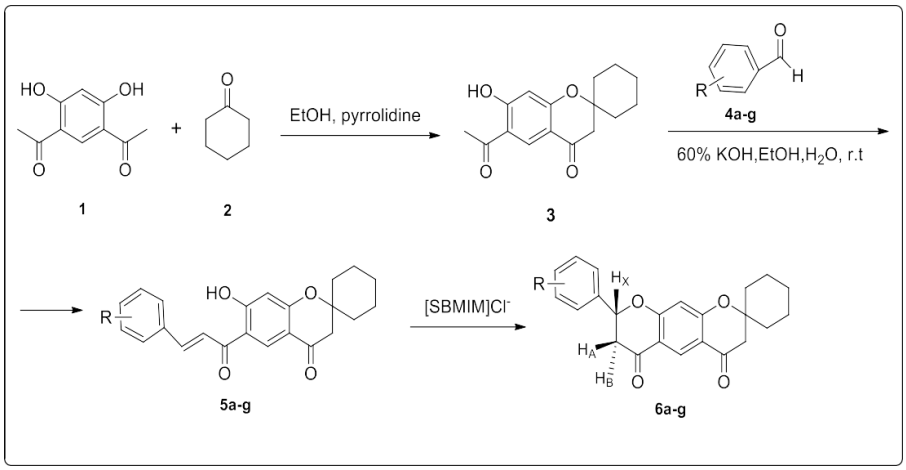
A) Preparationof6-(3-arylprop-2-enoyl)-7-hydroxyspiro-[chromane-2,1'-cyclohexan]-4-ones (5a–g).

A solution of 6-acetyl-7-hydroxy-spiro[chromane-2,1'-cyclohexan]-4-one (3) (260 mg,0.001mol)andsubstitutedbenzaldehyde4a–g(0.001mol) in ethanol (10ml)was added to a60% aqueous KOH solution(10 ml) at 0°C and stirred at room temperature while monitoring the reaction by TLC. After completion of reaction, the reaction mixture was acidified to pH ~4 by using dilute aqueous 2 N HCl solution to precipitate the product as yellow solid which was then recrystallized from ethanol. (Table 1).

B) Preparationof8'-aryl-7',8'-dihydro-6'H-spiro[cyclohexane-1,2'pyrano[3,2-g] chromene]-4',6' (3'H)-diones (6a–g).

A chalcone derivative 5a–g (200 mg, 0.55 mmol) was dissolved in ethanol (10 ml) using TSIL [SBMIM]Cl^- as acidic catalyst and heated under reflux for 3 h. After completion of reaction, to the crude residue, dichloromethane was added, and the solution was extracted with 10% NaHCO3 solution followed by brine and catalyst was recovered by using simple filtration. The concentrated organic layer was purified by column chromatography using petroleum ether – AcOEt, 9:1, as eluent.(Table 2).



Scheme1: Synthesisof8'-aryl-7',8'-dihydro-6'H-spiro[cyclohexane-1,2'- pyrano[3,2-g]chromene]-4',6'(3'H)-diones.

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Table1: Synthesisconditionsandyieldsofcompounds5a–g

Entry	R	Time(hr)	Yield(%)	M.P(^{0}C)
5a	H	3	94	151-153
5b	4-F	1.5	91	155-156
5c	4-Cl	2	92	152-154
5d	4-Br	2	95	153-155
5e	4-Me	3	92	157-159
5f	4-MeO	1.5	91	163-164
5g	3,4,(MeO)2	3	94	186-188

Table2:Synthesisconditionsandyieldsofcompounds6a–g

Entry	R	Time(hr)	Yield(%)	M.P(^{0}C)
6a	H	2.5	92	131-132
6b	4-F	1	90	139-141
6c	4-Cl	1.5	92	155-157
6d	4-Br	2	95	161-162
6e	4-Me	2.5	93	134-135
6f	4-MeO	2	91	129-131
6g	3,4,(MeO)2	2.5	93	130-132

Spectral data:

5a) 6-Cinnamoyl-7-hydroxyspiro[chromane-2,1'-cyclohexan]-4-one:

Yellowsolid;m.p.151–153°C;

IR(KBr):3422,1695,1634,1612,1368cm^{-1}

1HNMR (200 MHz,CDCl3):δ13.56 (s,1H);8.58(s,1H);7.95(d,1H,J=15.8);

7.72–7.70 (m, 2H); 7.68 (d, 1H J =15.8); 7.48–7.46(m, 3H); 6.52 (s, 1H); 2.74 (s, 2H); 2.03–1.97 (m, 2H) ; 1.76–1.54 (m, 8H). Mass(m/z):363 [M+H]$^+$

5b)(E)-6-[3-(4-fluorophenyl)prop-2-enoyl]-7-hydroxyspiro-[chromane- 2,1'cyclohexan]-4-one:

Yellowsolid;m.p.155-156°C;

IR(KBr):3370,1692,1639,1618,1369cm^{-1};

1HNMR(200MHz,CDCl3):δ13.52(s,1H); 8.56(s,1H);7.90 (d,1H,J=15.8);

7.72–7.68 (m, 2H);7.60 (d, 1H, J= 15.8);7.18–7.14 (m, 2H);6.53 (s, 1H);2.73 (s, 2H); 2.03–1.99 (m, 2H); 1.75–1.50 (m, 8H)., Mass(m/z):379 [M+H]$^+$

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5e)(E)-7-Hydroxy-6-[3-(p-tolyl)prop-2-enoyl]spiro[chromane2,1'-cyclohexan]-4- one:

Yellowsolid;m.p.157-159°C;

IR(KBr):3422,1694,1634,1612, 1368cm^{-1};

1HNMR(200 MHz,CDCl3):δ13.63(s,1H);8.56(s,1H);7.91 (d,1H,J=15.2);

7.63(d, 1H,J=15.2);7.59(d,2H,J=8.4);7.26(d,2H,J=8.4);6.50(s,1H);2.72

(s,2H);2.41(s,3H);2.01–1.98(m,2H);1.76–1.50 (m,8H). Mass(m/z):375 [M+H]$^+$

6a)8'-Phenyl-7',8'-dihydro-6'H-spiro[cyclohexane-1,2'-pyrano[3,2-g]chromene] 4', 6' (3'H)-dione:

Yellow solid; m.p. 131-132 °C; IR(KBr):1696,1608,1368cm^{-1}

1HNMR(200MHz,CDCl3):δ8.56(s,1H);7.48–7.39(m,5H);6.58(s,1H);

5.52(dd,1H,dd,JXB= 12.6,JXA= 3.1);3.03(dd,1H,JAB=16.9,JBX=12.6)and

2.92 (dd, 1H, JAB= 16.9, JAX= 3.2); 2.70 (s, 2H); 1.98–1.97 (m, 2H); 1.78–1.54 (m, 8H).

Mass(m/z):363 [M+H]$^+$

6b)8'-(4-Fluorophenyl)-7',8'-dihydro-6'H-spiro[cyclohexane-1,2'-pyrano[3,2 g]chrom- ene]-4',6'(3'H)-dione:

Yellow solid; m.p. 139-141 °C; IR(KBr):1696,1607,1374cm^{-1}

1HNMR(200MHz,CDCl3):δ8.56(s,1H); 7.48–7.44(m,2H); 7.16–7.12 (m,2H

);6.58(s,1H);5.49(dd,1H,JXB=12.6,JXA=3.1);3.04(dd,1H,JAB=16.7,JBX=

12.6);2.89(dd,1H,JAB=16.9,JAX=3.0);2.72(s,2H);1.98–1.96(m,2H);

1.76–1.53(m,8H). Mass(m/z):379 [M+H]$^+$

6e)8'-(p-Tolyl)-7',8'-dihydro-6'H-spiro[cyclohexane-1,2'-pyrano[3,2- g]chromene]-4', 6' (3'H)-dione:

Yellow solid; m.p. 134-135 °C; IR(KBr):1695,1606,1368cm^{-1}

1HNMR(200MHz,CDCl3):δ8.54(s,1H);7.55(d,2H,J= 7.9);7.25(d,2H,J=

7.9);6.55(s,1H);5.47(dd,1H,JXB=12.8,JXA=3.0);3.06(dd,1H,JAB=16.7,

JBX=12.8);2.87(dd,1H,JAB=16.7,JAX=3.0);2.70(s,2H);2.38(s,3H);1.98–

1.95 (m,2H);1.72–1.51(m,8H). Mass(m/z):375 [M+H]

Result and Discussion:

A three-step synthetic strategy chromanone–chalcone–pyranoflavanone was followed as outlined in **Scheme 1**. 4,6-Diacetylresorcinol **(1),** prepared according to literature procedure,[13-15] undergo the Kabbe condensation with cyclohexanone in the presenceof pyrrolidine as a base in refluxing ethanol providing spirochromanone derivative **3**[16] in 62% yield. In the next step, Claisen–Schmidt condensation of compound **3** with various aryl aldehydes **4a–g** produced spiropyran-annulated chalcones **5a–g** in good yields (91–95%) under reflux condition(2.5-1 hr, method B), and no side products were detected **(Table 1).**Lastly, it was found that chalcones **5a–g** can be easily cyclized to

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flavanones **6a–g** in excellent yields in presence of TSIL [SBMIM]Cl^- in excellent yield as compared to traditional catalyst [17-20]**(Table 2).**The structure of all synthesized products, **5a–g, 6a–g** was confirmed by IR, ^1H NMR and mass spectral analysis. For example, the IR spectrum of compound **5a** showed absorption bands at 3420, 1693, and 1632 cm^{-1} due to the O–H, C=O, and α,β- unsaturated ketone (cinnamoyl) C=O groups, respectively. In the mass spectrum of compound **5a** the base peak appeared at m/z 363 corresponding **5a,** as a characteristic example for the whole series **5a–g,** a two-proton singlet at2.72ppmassignedtothe3- CH_2group of the chromanone skelet on was detected. More, the appearance of a sharp singletat13.54ppminthe^{1}HNMRspectrum, suggested the presence of ahydroxyl group involved in a hydrogen bond. In addition, the coupling constant for olefinic protons was about 15 Hz indicating the trans configuration for the chalcone C=C double bond. In the IR spectrum of compounds **6a,** the band due to the C=Ostretching of flavanones **6a–g** occurred at 1602–1610 cm^{-1}. Inthe ^1H NMR spectrum of flavanone **6a,** there were three doublets of doublets at 5.51, 3.02, and 2.90 ppm.The pattern of these peaks was characteristic of an ABX spin system of protons located at positions 2 and 3 of a chromane ring with aromatic substitution. The formation of a new pyran ring is thus confirmed by the presence of ABX systemin ^1H NMR spectrum due to the observed geminal and vicinal coupling between protons H_A, H_B, and H_X **(Scheme 1).** The H_A and $H_B$protons (7'-CH_2 of the pyranochromane system) differ in coupling constant values with the proton H_X(8'-CH) and, hence, are anisogamous, the $H_A$proton being cis-oriented(J_{AX}=3.0Hz) and the H_B proton being trans-oriented(J_{BX}= 12.5 Hz)relative to the $H_X$proton. The 7'-CH2 protons mutually interacted with a geminal coupling constant J_{AB}=16.8 Hz. All the other signals from NMR spectra are in agreement with the proposed structures.

Hence, the use of acidic TSIL [SBMIM]Cl^- offers a clean and cheaper alternative catalyst to the conventional catalyst, indicating that the by using [SBMIM]Cl^-makes reaction to occur at shorter reaction times in goodyields for cyclization ofchalcones **5a–g** cyclized to flavanones **6a–g**. The structure of all synthesized products **3**, **5a–g, 6a–g** was confirmed by IR, ^1H NMR and mass spectral analysis.

Conclusion:

In conclusion, here in we report simple and an efficient method for the synthesis of spirochromanone–flavanone hybrid molecules from spirochromanone–chalcone hybrids by the use of TSIL[SBMIM]Cl^- asan in expensive and safe acid catalyst. This protocol will be a good addition to the most recent environmentally friendly methods reported for the synthesis of flavanones. The spirochromanone–chalcone hybrid molecules were synthesized under eco friendly condition. The merits of this method are the use of inexpensive and reusable catalyst, as well as easy workup and purification procedure. The high yields and short reaction times make this approach an interesting alternative to the existing methods.

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Microwave Assisted and Eco-friendly synthesis of pyridine based Chalcone and its derivatives

Aiyanile N.B., Tekale A.S, Reddy P.S., Muley D.B.
Chemistry Department, PG students in Shivaji Mahavidyalya Udgir, (MH)-413517
Email: akankshamane13928@gmail.com, reddypravin50@gmail.com

Abstract:

Now in a current scenario green approach in organic synthesis covers a precious value over its traditional one. Green synthesis evolving in this decade got an appreciation from many researchers. This method for the synthesis of derivative of Prop-2en-1one from 2- acetyl pyridine and different aromatic aldehyde at room temperature by using PEG-400 solvent under microwave irradiation yields chalcone within short of time with excellent yield. This method is suitable alternative path for the green approach. In this method may consider as convenient route for synthesis of Chalcone derivative.
Keywords- 2-acetyl pyridene, PEG-400, microwave irradiation, chalcone

1. Introduction:

In the last decade Chalcone derivative got enormous value due to its pharmaceutical importance.It may find the application as precursor for the synthesis of many organic compounds. Chalcone is useful for its pharmacological activities. Many organic compounds such as flavonoid1, isoflavonoid2, pyrazole, pyrimidine etc are synthesized from chalcone derivatives. Chalcone find its importance in various biological applications comprising anti-inflammatory3-4, antiviral5, anti depressant6, anti-bacterial7, anti-tumor8, anticancer 9-12, antileishmanial13, immunomodulatory14, ant hyperglycemic 15, antiangeogenic activities16. In this study the synthesis formation of prop-2-en-1-one from 3-acetyl pyridine and different aromatic aldehyde in presence of strong alkali with PEG -400 as a green solvent under microwave irradiation shows extraordinary result with excellent yield of product. In the recent time microwave irradiation was spontaneously getting importance in the field of organic synthesis. The process is simple and convenient and the use of polyethylene glycol -400 proved to be ecofriendly. We attempt to synthesize Prop-2en-1- one derivative by using principles of green chemistry. The solvent taken PEG- 400 considered as environmental benign reaction solvent. It is easily available, water soluble, nontoxic, and cheap in cost from which separation of reaction product facilate. In addition to their numerous biological activities, chalcones find a pronounced application in synthetic organic chemistry. Many heterocyclic compound are synthesized by using chalcone and as synthons for the synthesis of many pharmaceuticals. Having such a varied pharmacological activity and synthetic utility, chalcones have attracted chemists to develop a large number of synthetic methodologies for their synthesis around the world.

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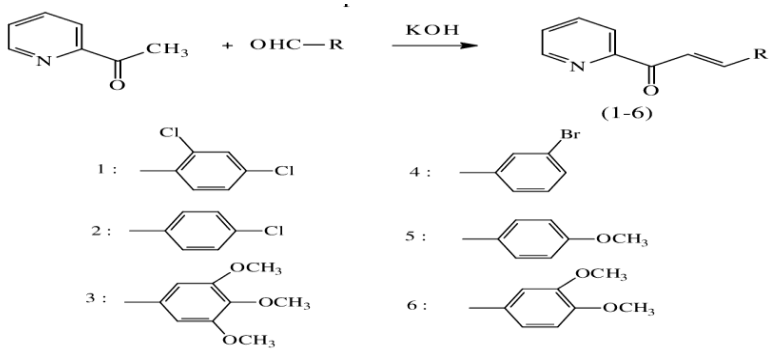
2. Material and Methods:

Experimental: The analytical grade chemicals are purchased. The synthesized product is crystallized with ethyl alcohol and the purity of synthesized compound is checked by thin layer chromatography. The melting point of compound is taken in an open capillary and is uncorrected. Infrared spectra were recorded on Perkin Elsmeir spectrometer. The 1H NMR spectra were recorded on 400 MHz spectrometer with TMS as an internal standard. The purification of compound is done by recrystallisation in ethyl alcohol. ProcedureA mixture of 2-acetyl Pyridene (0.01 mole) and aromatic aldehyde (0.01 mole) were mixed well in 20 ml of PEG-400 and then Aq. 30% KOH was added drop wise with continuous stirring and shaken well. The reaction mixture was put under microwave irradiation for 2-3 minutes. The completion of reaction was checked by thin layer chromatography. After confirmation of completion of reaction, complete reaction mixture was poured into crushed ice and acidified with HCl if necessary in order to maintain PH. The solid precipitate obtained was filtered and recrystallised from ethanol. The characterization of synthesized organic compound is completed.



Scheme 1. Synthesis of chalcones of 2-acetyl pyridine

Table 1. Physical data of compounds **(1-6)**

Compd.	M.F.	M.P. °C	Yield, %	Elemental analyses, % C Found	C Calcd	H Found	H Calcd.	O Found	O C
1	$C_{14}H_9ONCl_2$	155	88	60.23	60.45	3.12	3.26	5.36	5.
2	$C_{14}H_{10}ONCl$	167	82	69.25	69.00	4.02	4.13	6.32	6.

IR –data (CM-1) :- 1 - 1721 (C=O), 1645 (CH=CH), 855 (C-Cl), 1512 (C=N) 2- 1724 (C=O), 1648 (-CH=CH), 851 (C-Cl), 1536 (C=N) 3- 1730 (C=O), 1652 (-CH=CH), 860 (C-Br), 1530 (C=N) 4- 1732 (C=O), 1651 (-CH=CH), 1174 (-OCH3), 1584 (C=N)

1H NMR (in ppm) Compound 1- 7.31 (1H, d, C-3' -H), 7.47 (1H, d, -CO-CH=), 7.57 (1H, d, C-6-H), 7.88 (1H, s, C-3-H), 7.92 (2H, m, C-4' -H, C-5' - H), 8.23 (1H, d, C-5-H), 8.32 (1H, d, =CH-Ar), 8.78 (1H, d, C-6' -H)

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Result and Conclusion: The synthesis of chalcone from 2-acetyl pyridene with different aromatic aldehyde under microwave irradiation by using PEG-400 solvent emerges out to be an eco-friendly and a clean product is obtained during synthesis with good percentage of yield. Acknowledgement The Authors are thankful to the Principal Dr. Vinayak Jadhav Of Shivaji College Udgir for providing research lab facility. The authors are also thankful to Asst. Prof. Swami Mantosh B., Head of Department chemistry of M.B. College Latur for providing consistent support in the field of synthesis.

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Thiophene Derived Schiff Base Ligand and Its Metal Complexes: An Overview

Yogesh N. Bharate[1], Kuldeep B. Sakhare[1], Kirti N. Sarwade[1], Mahadeo A. Sakhare[1*]
[1*]Dept. of Chemistry, Balbhim Arts, Science & Commerce College, Beed Maharashtra-431122.

Abstract:

Thiophenederived Schiff base ligands are known to show various biological activities and if these Schiff base ligands are coordinated with corresponding metal complexes then their activity ratio increases with twice or more. Especially if the Schiff base ligands are coordinated with Cd(II), Cu(II), Zn(II) etc. are reported to show greater biological activities as compared to other transition metals. In this review article we have given the confirmative data of Schiff base ligand like mass spectra, ^{1}H-NMR spectra, FTIR spectra and that of metal complexes like powder XRD, thermogravimetric analysis, FTIR etc. also we have given some biological activities like anti-bacterial, anti-fungal, anti-cancer and compared Schiff base ligand with corresponding metal complexes against some standard drugs.

Keywords: Thiophene, Metal Complex, Spectroscopy, Thermogravimetry.

1. Introduction:

From the last three decades various diseases are disturbing the whole human life style by their hazardous effects. Scientists as well as researchers are busy to finding the solution on it. Finding of new effective drug is very needful in these days. The Coordination chemistry which is branch of inorganic chemistry is playing important vital role in this research area as it has broad peak of biological activities.

In 1864 Hugo Schiff was discovered the compound by condensing aldehyde with primary amine and found very active in various fields. For his novel discovery he has been awarded by noble prize at that time and the compound formed by the condensation of aldehyde and amine is commonly known as Schiff base ligand. In the discovery of new potential drugs against various diseases Schiff base ligands are widely used by Scientist as well as researchers as it shows broad spectrum of various biological activities such as: antifungal,antibacterial,anti-HIV, antiviral, anticonvulsant, antioxidant, antidiuretic, antimalarial, analgesic, antituberculosis, antitumor, anti-ulcer, anthelmintic, anti-inflammatory, antiprotozoal, anti-Alzheimer, anti-hypertension, herbicidal properties have made them more and more important [1-13].

In the addition to Schiff base ligand it metal ions are coordinated by the donor hetero(O/N/S) atoms, which are present in the Schiff base ligand then the peak of all the biological activities increases such

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as: antimicrobial, anticancer[14]. Because of this reason researchers are attracted towards the synthesis of Schiff base ligand along with their metal complexes. Thiophene is one of the most popular amine in the field of Schiff base chemistry as it has heteroatoms Sulphur and Nitrogen in its moiety. The nitrogen atom donates the loan pair of electron to the metal ions and make the metal complexes stable and potentially active in biological activities.

2. Experimental:

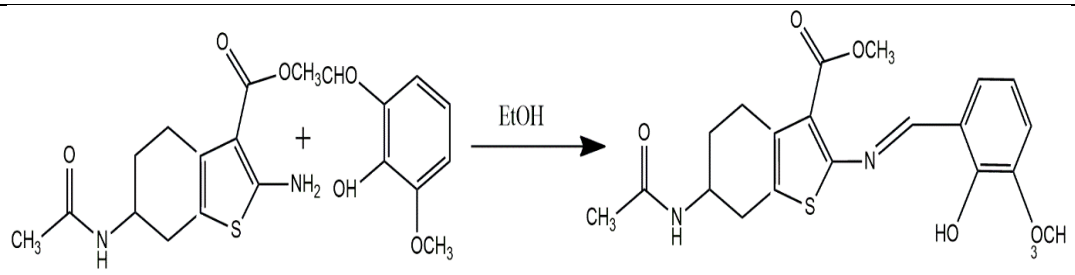
2.1 Synthesis of Schiff base ligand and metal complexes:

For the synthesis of Schiff base ligand of Thiophene based amine is quite easy, as it is cheap and readily available. The various methods can be utilised for the synthesis of Schiff base ligand such as reflux method, via green approach etc. following are given some of the method of synthesis.

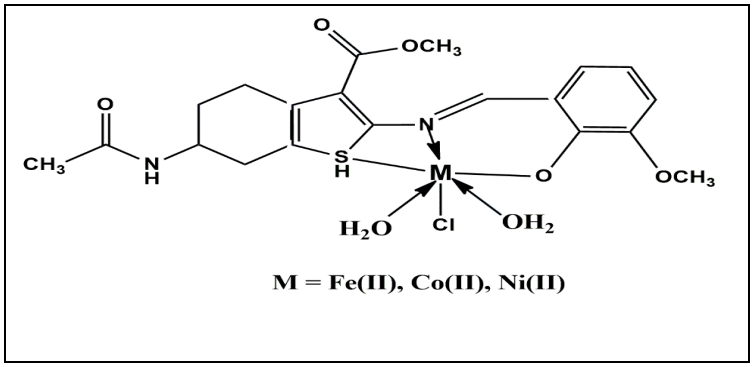
Mustafa Bingöl and NevinTuran[15] Prepared the Schiff base ligand pf thiophene based amine along with metal complexes and evaluated this against various biological activities such as: antioxidant activity, antibacterial activity, antifungal activity. In this article they observed that metal complexes exhibit superior activity than that of Schiff base ligand. The structure of Schiff base ligand and metal complexes is shown the scheme 1 and scheme 2:

Scheme 1: Synthesis of Schiff base ligand.

Scheme 1: Synthesis of Schiff base ligand.



Scheme 2: Synthesis of Metal Complexes.



Scheme 2: Synthesis of Metal Complexes.

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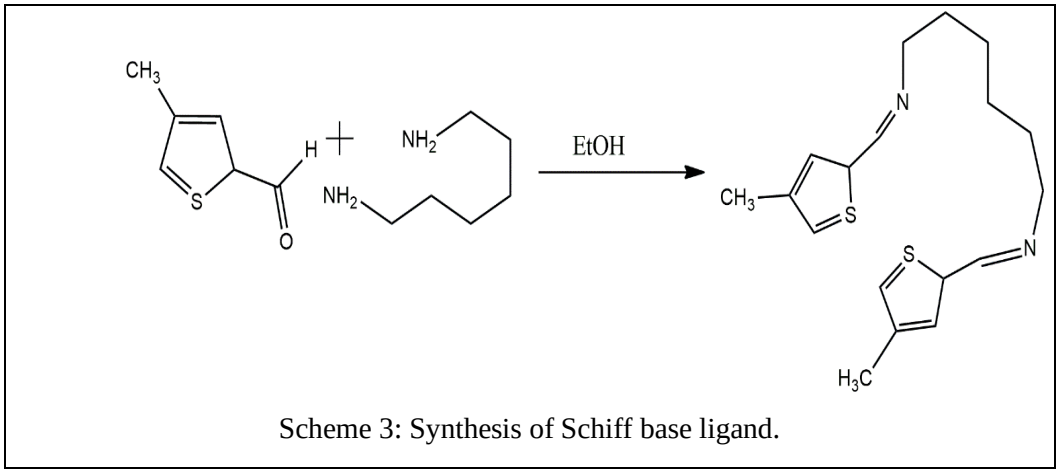
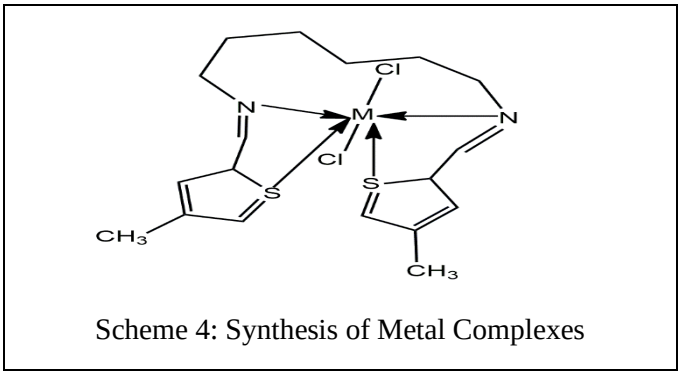
GühergülUluçamet al.,[16] has synthesized the Schiff base ligand and its metal complexes. Further his team has evaluated these compounds with various biological activities such as: Antibacterial, Antifungal, Anticancer etc. in these observations they concluded that the metal complexes shows better activities than that of Schiff base ligand. The synthesis of Schiff base ligand and metal complexes is illustrated in scheme 3 and 4 respectively.

Scheme 3: Synthesis of Schiff base ligand.



Scheme 3: Synthesis of Schiff base ligand.

Scheme 4: Synthesis of Metal Complexes.



Scheme 4: Synthesis of Metal Complexes

Rajesh Malhotra and Ankit Ravesh[17] have prepared the Schiff base ligand based on Thiophene-22carboxylic acid and 2-benzyloxy-3-methoxy-benzaldehyde. They also synthesized metal complexes. After the preparation of these compounds they have tested it against antifungal and antibacterial activities. In this result they observed that metal complexes shows higher activities than that of Schiff base ligand. The scheme 5 and 6 represents the synthesis of Schiff base ligand and metal complex as follow.

Scheme 5: Synthesis of Schiff base ligand.

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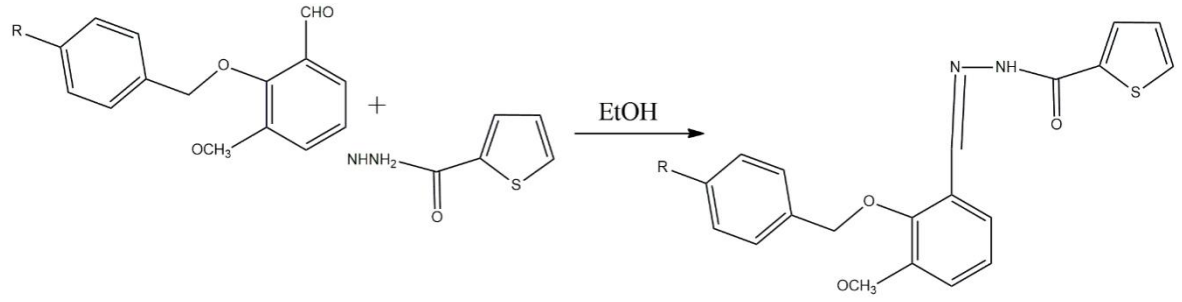
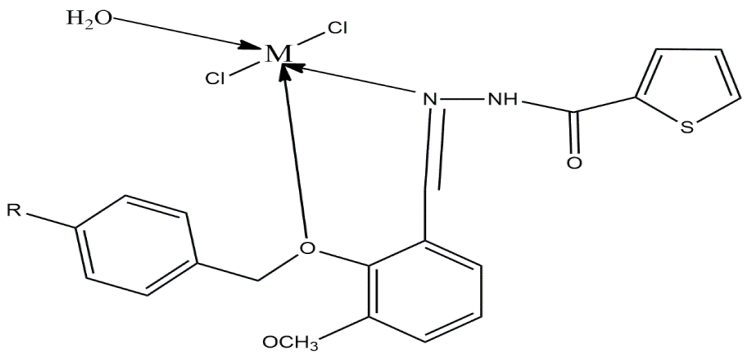


Scheme 5: Synthesis of Schiff base ligand

Scheme 6: Synthesis of Metal Complexes.



Scheme 6: Synthesis of Metal Complexes.

Amit kumar[18] have synthesized the Schiff base ligand and its metal complexes. Further he has evaluated these compounds with antibacterial activities. In this activity he found that the metal complexes shows greater activity than the Schiff base ligand.

3. Conclusion:

In this review article we have focused the synthesis of Schiff base ligand based on the Thiophene and its transition metal complexes. After a broad literature survey it is clear that Schiff base ligand shows good biological activities but if metal salts are coordinated with this then the graph of all these activities get enhances. We can also conclude that there is large scope for the research in the field of coordination chemistry by synthesising various Schiff base ligand by Thiophene as it is readily available and cheap in price but shows very good activities. It can be helpful for synthesising novel drugs against various diseases.

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Imidazole a Pharmaceutical Significant molecule: A Review

Arshia Parveen[1], Daimi Asma Anjum[2]

[1]*Department of Chemistry, B. Raghunath ACS College, Parbhani-431401.MS.India*
[2] *Department of Chemistry, Shri Shivaji College, Parbhani-431401.MS.India*
Email: daimiasmaanjum@gmail.com arshiairfanmalik@gmail.com

Abstract:

Imidazole is a five-membered heterocyclic moiety that possesses three carbon, two nitrogen, four hydrogen atoms, and two double bonds. It is also known as 1, 3-diazole. It contains two nitrogen atoms, in which one nitrogen bear a hydrogen atom, and the other is called pyrrole type nitrogen. Imidazole was first synthesized by Heinrich Debus in 1858 and was obtained by the reaction of glyoxal and formaldehyde in ammonia, initially called glyoxaline. The current literature provides much information about the synthesis, functionalization, biological role of imidazole and commercially available drugs containing imidazole nucleus. Imidazole is a structure that, despite being small, has a unique chemical complexity. It is a nucleus that is very practical and versatile in its construction/functionalization and can be considered a rich source of chemical diversity. Imidazole acts in extremely important processes for the maintenance of living organisms, such as catalysis in enzymatic processes. Imidazole-based compounds with antibacterial, anti-inflammatory, antidiabetic, antiparasitic, antituberculosis, antifungal, antioxidant, antitumor, antimalarial, anticancer, antidepressant and many others make up the therapeutic arsenal and new bioactive compounds proposed in the most diverse works. The interest and importance of imidazole-containing analogs in the field of medicinal chemistry is remarkable, and the understanding from the development of the first blockbuster drug cimetidine explores all the chemical and biological concepts of imidazole in the context of research and development of new drug.

Keywords: imidazole; synthesis; medicinal chemistry; drug discovery

1. Introduction:

Nowadays, Public health problems were increasing due to AMR in drug therapy. So, there is necessary for the development of a new drug that overcomes the AMR problems [1]. In past, those drugs which contain heterocyclic nuclei give high chemotherapeutic values and act as a remedy for the development of novel drugs [2]. Tere are lots of heterocyclic compounds that are in clinical use to treat infectious diseases. So, there is a great importance of heterocyclic ring containing drugs [3]. In heterocyclic chemistry, imidazole containing moiety occupied a unique position [4]. It is a fve-membered nitrogenous heterocyclic moiety that possesses three carbon, two nitrogen, four hydrogen atoms, and two double bonds having general molecular formula is C3H4N2 (Fig. 1). Te nitrogen atoms present at the frst and third positions (non–adjacent position) of the ring [5], position four and fve are equivalent [6]. It is also known as 1,3-diazole. It contains two nitrogen atoms, one nitrogen bear a hydrogen atom, and the other is called pyrrole type nitrogen [7]. 1,3-diazole ring is a bioester of the pyrazole ring [8]. It is the basic core of some natural products such as histidine, purine, histamine and DNA based structures, etc. [4]. Te imidazole name was frst reported by Arthur Rudolf Hantzsch (1857–1935) in 1887 [6]

1,3-diazole shows an amphoteric phenomenon i.e. it can behave like acid as well as a base. Two types of lone pair are present in the imidazole ring, delocalized and non-delocalized (non-

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Huckle) lone pair, i.e. both nitrogen of 1,3-diazole shows diferent dissociation constant. Te dissociation constant (pKa) of delocalized lone pair and non-delocalized lone pair is 7 and 14.9 respectively. 1,3-diazole ring is susceptible to both electrophilic and nucleophilic attacks due to its amphoteric phenomenon [7]. For an acid imidazole, the dissociation constant is 14.5, which makes it less acidic than phenol, imides, and carboxylic acid except for alcohols (which is less acidic than imidazole). For a basic imidazole, the dissociation constant (pKa) is approximately 7 (which makes imidazole 60 times more basic than pyridine). Te acidic proton is present on the frst nitrogen atom of the imidazole ring [6]. Due to the presence of a positive charge on either of the two nitrogen atoms, 1,3-diazole ring shows two equivalent tautomeric forms (Fig. 2) [9]. Te presence of a sextet of π-electrons on the ring makes it an aromatic compound. Te nitrogen atom on the third position in the imidazole ring is more reactive to the electrophilic compound due to the availability of unshared pairs of electron on the second nitrogen atom since the second nitrogen is a part of aromatic sextet [6]. It is a white or colorless solid. Te imidazole ring shows excellent solubility in water and other polar solvents [10]. Te dipole moment, melting point, and boiling point of the imidazole ring is 4.8 D in dioxane [6], 88.9 °C, and 267.8 °C [7] respectively.

It possesses intramolecular hydrogen bonding [9]. Imidazole was frst named glyoxaline because the frst synthesis has been made by glyoxal and ammonia [9]. Tere is a diferent kind of synthetic route from which we can synthesize 1,3-diazloes, and its derivatives. Common methods are Debus-Radiszewski synthesis, Wallach synthesis, from dehydrogenation of imidazolines, from alpha halo-ketones, Marckwald synthesis, and amino nitrile [11]. Due to the polar nature of the imidazole ring, the pharmacokinetic parameters of the imidazole containing compounds should be improved to a great extent. Tus, this moiety helps to overcome the solubility problems of poorly soluble drug entities [12]. Te 1,3-diazole and it's containing compounds shows a lot of therapeutic activities such as analgesics, antifungal, antihypertensive, antiobesity, antitumor [3], antiviral, anthelmintic, antitubercular [4], antiulcer, antihistaminic [13], anti-infammatory, antidepressant [14]. antidiabetic [15], anticonvulsant [16], antiallergic [7], antirheumatic [17], antiasthmatic, alpha-blockers [18], antiprotozoal [19], antiaging, anticoagulant, antimalarial [20], and antiamoebic activity [21] etc. Tere are diferent examples of commercially available drugs which consist 1,3,4-oxadiazole ring (Table 1) such as clemizole (antihistaminic agent), etonitazene (analgesic), enviroxime (antiviral), irtemazole, astemizole (antihistamine), omeprazole, pantoprazole (antiulcer), thiabendazole (antihelmintic), nocodazole (antinematodal) [22], metronidazole and nitrosoimidazole (bactericidal), megazol (trypanocidal) [12], azathioprine (anti-rheumatoid arthritis), tinidazole, ornidazole (antiprotozoal and antibacterial), satranidazole (amoebiasis), cimetidine (gastric ulcer), carbimazole (against thyroid disorder), tolazoline (vasodilator action), naphazoline (vasoconstrictor), tetrahydrozoline (vasoconstrictor) [16], etomidate, lansoprazole, fumazenil, methimazole, pilocarpine [19], ketoconazole [23], dacarbazine (anticancer) [24], pimobendan (calcium sensitizer and phosphodiesterase inhibitor) [25], fenbendazole [26].

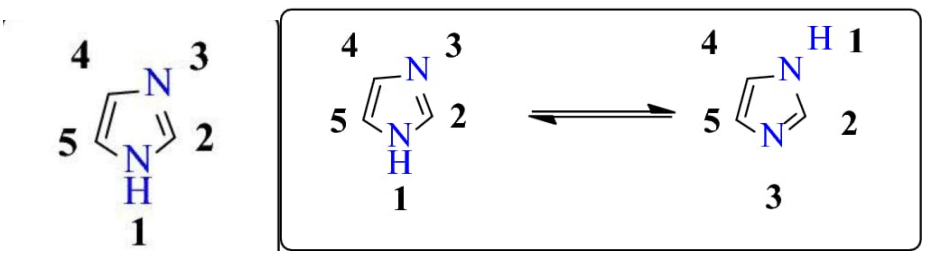

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Fig 1. imidazole fig2. Tautomeric forms of imidazole

Commercially available drugs are containing Imidazole nucleus

1] Clemizole

Upon oral administration, clemizole binds to and blocks the H1 receptor, thereby preventing the interaction between histamine and the H1 receptor and inhibiting H1-mediated signaling. This may inhibit or prevent the symptoms that are caused by histamine activity and rescues or prevents allergic reactions.[13]

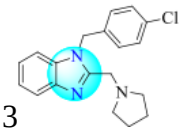

Fig.3

2] Etonitazene

Etonitazene and its related opioid agonist benzimidazoles were discovered in the late 1950s,[5][6][7][8][9][10] by a team of Swiss researchers working at the pharmaceutical firm CIBA (now Novartis). One of the first compounds investigated by the Swiss team was 1-(β-diethylaminoethyl)-2-benzylbenzimidazole, which was found to possess 10% of the analgesic activity of morphine when tested in rodent bioassays.[22]

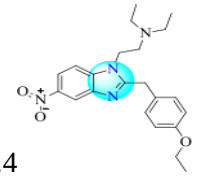

Fig.4

3] Enviroxime

Enviroxime is a substituted benzimidazole derivative with activity against rhinoviruses and enteroviruses. [4]

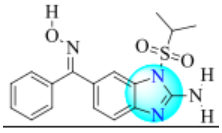

Fig.5

4] Irtemazole

It is used for promotion of uric acid i.e.***It*** is a uricosuric agent exhibiting a rapid uricosuric effect in normouricemic as well as in hyperuricemic persons.22

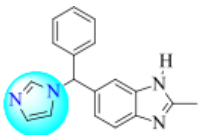

Fig.6

5] Astemizole

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It is an antihistamine. Antihistamines prevent sneezing, runny nose, itching and watering of the eyes, and other allergic symptoms. Astemizole is used to treat allergies, hives (urticaria), and other allergic inflammatory conditions.[13]

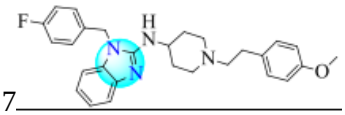

Fig.7

6] Omeprazole

It reduces the amount of acid your stomach makes. It's widely used to treat indigestion and heartburn, and acid reflux. It's also taken to prevent and treat stomach ulcers.[13]

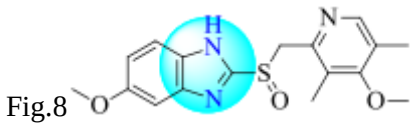

Fig.8

7] Pantoprazole

It is used to treat damage from gastroesophageal reflux disease (GERD), a condition in which backward flow of acid from the stomach causes heartburn and possible injury of the esophagus (the tube between the throat and stomach) in adults and children 5 years of age and older.[13]

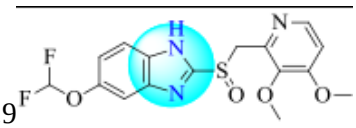

Fig.9

8] Thiabendazole

It is an antihelmintic drug that inhibits a specific enzyme of helminths, fumarate reductase, and is effective against a broad spectrum of nematode infections.[4]

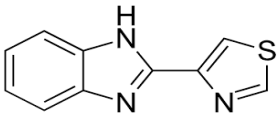

Fig.10

9] Nocodazole

Nocodazole is an anti-mitotic agent that reversibly interferes with the polymerization of microtubules. (De Brabander et al.). Nocodazole binds to beta-tubulin and disrupts microtubule assembly/disassembly dynamics, impairing formation of the metaphase spindles during the cell division cycle.[22]

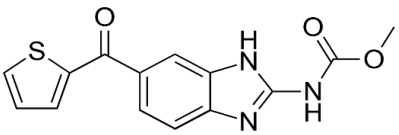

Fig.11

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10] Metronidazole

Metronidazole is used to treat infections of the reproductive system, gastrointestinal (GI) tract, skin, heart, bone, joint, lung, blood, nervous system, and other areas of the body. It is also used to treat certain sexually transmitted diseases (STDs).[16]

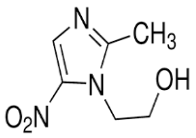

Fig.12

11] Nitroso imidazole

An imidazole antifungal used to treat vulvovaginal candidiasis. A broad spectrum antifungal used to treat seborrheic dermatitis and fungal skin infections. A topical antifungal used to treat tinea pedis, tinea cruris, tinea corporis, cutaneous candidiasis and tinea versicolor.[16]

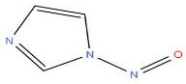

Fig.13

12] Megazol

Megazol (CL 64855) is a nitroimidazole based drug that cures some protozoan infections. Megazol A study of nitroimidazoles found the drug extremely effective.[12]

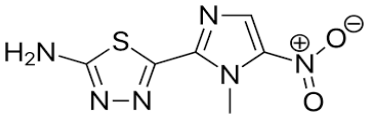

Fig.14

13] Azathioprine

Azathioprine (Imuran®) is a medication that treats diseases that have to do with your immune system. It's been used in some patients with multiple sclerosis (MS), usually if they have problems with standard FDA-approved medications for their MS.[16]

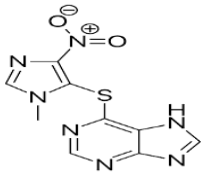

Fig.15

14] Tinidazole

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Tinidazole is used to treat infections caused by protozoa (eg, trichomoniasis, giardiasis, and amebiasis). It is also used to treat adult women with vaginal infections (bacterial vaginosis). Tinidazole belongs to the group of medicines called antiprotozoals.[28]

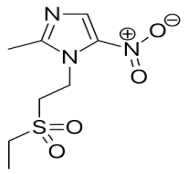


Fig.16

15] Ornidazole

Ornidazole is a synthetic nitroimidazole that is used to treat infections caused by anaerobic bacteria and protozoa. It can be prescribed for genitourinary tract infections and has been associated with dermal fixed drug eruptions in some cases.[28]

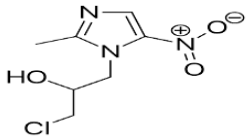


Fig.17

16] Satranidazole

Satranidazole belongs to a group of medicines known as antibiotics used to treat various infections caused by bacteria and parasites (amoeba). It is prescribed for the treatment of diarrhea. Additionally, it also treats vaginal and other bacterial infections.[16,21]

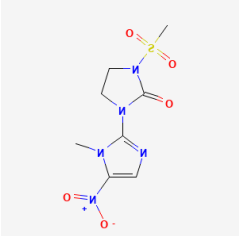
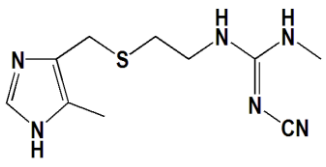


Fig.18

17] Cimetidine

Cimetidine is used to treat ulcers; gastroesophageal reflux disease (GERD), a condition in which backward flow of acid from the stomach causes heartburn and injury of the food pipe (esophagus); and conditions where the stomach produces too much acid, such as Zollinger-Ellison syndrome.[13]



Cimetidine

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Fig.19

18] Carbimazole

It is a medicine used to treat an overactive thyroid (hyperthyroidism). This is when your thyroid gland makes too many thyroid hormones.[16]

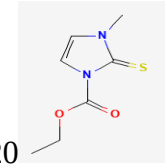

Fig.20

19]Tolazoline

Tolazoline is a nonselective vasodilator that has been used for several decades to treat pulmonary hypertension in neonates. Its primary action appears to be as a competitive α-adrenergic antagonist.[16]

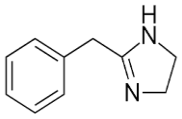

Fig.21

20] Naphazoline

It is used to relieve redness due to minor eye irritations, such as those caused by colds, dust, wind, smog, pollen, swimming, or wearing contact lenses. Some of these preparations are available only with your doctor's prescription.[16]

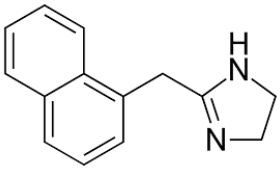

Fig.22

21] Tetrahydrozoline

It is a decongestant used to relieve redness in the eyes caused by minor eye irritations (suchas smog, swimming, dust, or smoke). It belongs to a class of drugs known as sympathomimetic amines. It works by temporarily narrowing the blood vessels in the eye. [16]

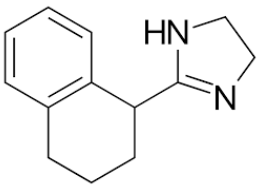

Fig.23

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22] Etomidate

It is a short-acting intravenous anesthetic indicated for the induction of anesthesia and supplementation of subpotent anesthesia during short operative procedures. Imidazole derivative anesthetic and hypnotic with little effect on blood gases, ventilation, or the cardiovascular system.[19]

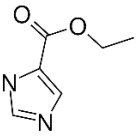

Fig.24

23] Lansoprazole

It's used for indigestion, heartburn, acid reflux and gastroesophageal-reflux-disease (GORD). Lansoprazole is also taken to prevent and treat stomach ulcers. Sometimes, lansoprazole is taken for a rare condition caused by a tumour in the pancreas or gut called Zollinger-Ellison syndrome.[13]

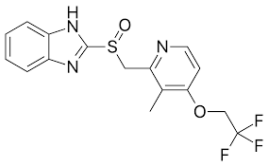

Fig.25

24] Flumazenil

Flumazenil is a benzodiazepine antagonist typically used in overdose emergencies. The primary FDA-approved clinical uses for flumazenil include reversal agents for benzodiazepine overdose and postoperative sedation from benzodiazepine anesthetics.[19]

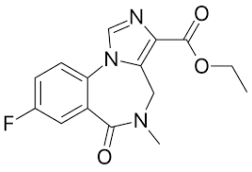

Fig.26

25] Methimazole

is a thionamide antithyroid agent that inhibits the synthesis of thyroid hormones.[6,14,12] It was first introduced as an antithyroid agent in 1949[2] and is now commonly used in the management of hyperthyroidism, particularly in those for whom more aggressive options such as surgery or radioactive iodine therapy are inappropriate.[16]

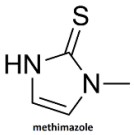

Fig.27

26] Pilocarpine

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It is a lactone alkaloid originally extracted from plants of the Pilocarpus genus.[4] It is used as a medication to reduce pressure inside the eye and treat dry mouth.[1][5] As an eye drop it is used to manage angle closure glaucoma until surgery can be performed, ocular hypertension, primary open angle glaucoma, and to constrict the pupil after dilation.[19]

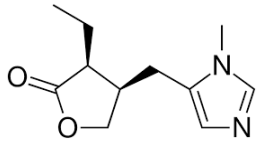

Fig.28

27] Ketoconazole

Itis an imidazole antifungal agent used in the prevention and treatment of a variety of fungal infections. [Label]. It functions by preventing the synthesis of ergosterol, the fungal equivalent of cholesterol, thereby increasing membrane fluidity and preventing growth of the fungus.[3]

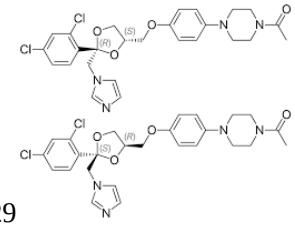

Fig.29

28] Dacarbazine

It is a chemotherapy drug. You pronounce dacarbazine as da-car-ba-zeen. It is also called DTIC. It is a treatment for several cancers that have spread (advanced cancer).[24]

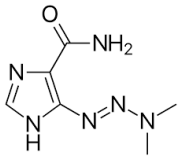

Fig.30

29]Pimobendan

Its (brand name Vetmedin®) is a heart medication used to treat dogs with congestive heart failure (CHF) usually caused by dilated cardiomyopathy or valvular insufficiency. Its use in cats to treat heart failure is off label (extra label).[25]

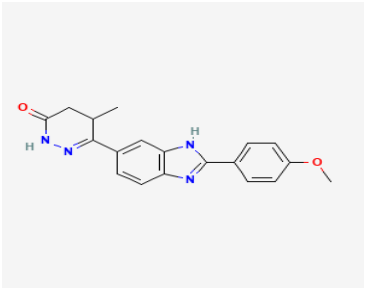

Fig.31

30] Fenbendazole

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Fenbendazole (brand names Panacur®, Safe-Guard®) is a medication used to treat a variety of parasites in dogs (e.g., roundworm, hookworm, lungworm, whipworm, and certain types of tapeworm). Its use in cats for the treatment of parasites is "off label" or "extra label".[22]

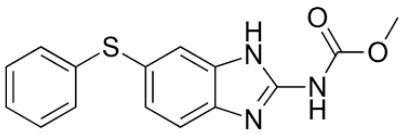

Fig.32

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Biochemical assessment of cestode parasites in fresh water fish *Mastacembelus armatus*

[1]Amol S. Thosar, [1]Suraj S. Kolhe, [1]Ravi V. Solunke
[1]Department of Zoology and Fishery Science, Dayanand Science College, Latur
Email- amol.thosar27@gmail.com

Abstract

Parasitic biochemistry is a growing field that has garnered increasing attention, particularly with the rising focus on tropical diseases. Over time, parasitologists have integrated biochemical methods to stay abreast of developments in the area. This research often involves examining biomolecules such as proteins, glycogen, and lipids within both parasites and the intestines of infected and non-infected hosts. Recent studies comparing the cestode parasite Senga sp. to the intestines of its hosts have uncovered notable findings. It was found that Senga sp. has lower levels of proteins and glycogen than both infected and non-infected host intestines. In contrast, lipid levels in *Circumoncobothrium* sp. are higher compared to those in the host intestines. Moreover, the concentrations of proteins, glycogen, and lipids are observed to be greater in non-infected intestines than in infected ones.

Keywords: Biochemical estimation, Cestodes, *Mastacembelus armatus*.

1. Introduction

Fish are often considered "gold in the water" because of their economic importance and their ability to provide high-quality protein to support a growing global population. However, malnutrition remains a pressing issue, and fish are not exempt from these challenges. A significant concern is the damage caused by tapeworm infections, which affect both fish and humans. Cestodes, or tapeworms, which reside in the digestive tracts of vertebrates, primarily rely on glucose as an essential energy source (Mishra et al., 1991). Studies have indicated that cestodes accumulate substantial carbohydrate reserves and are efficient in metabolizing these reserves (Daugherty, 1966; Fairbairn et al., 1961; Markov, 1939; Read & Rothman, 1957). It is widely accepted that the stored carbohydrates in these parasites are primarily in the form of glycogen (Read, 1949). Proteins are essential for a wide range of biological functions and are found throughout various organisms. Despite their critical roles, there is no single, universally agreed-upon system for classifying proteins. Enzymes represent one of the largest categories of proteins and serve as an important nutritional source for cestodes (tapeworms). These parasites rely on varying amounts of protein to generate energy. Literature suggests that cestodes can only thrive in a parasitic environment when protein, which typically makes up 20–40% of their dry weight, is present (Barrett, 1981). Furthermore, research has shown that lipid concentrations tend to rise in older proglottids, the segments of tapeworms (Brand & Van T., 1952). he glycogen content in various helminths can vary considerably depending on their environment, even though their nutritional requirements may differ. For cestodes, which inhabit the digestive tracts of vertebrates, glucose serves as a critical energy source (Mishra et al., 1945). These parasites have a significant ability to store and metabolize carbohydrates. Studies have shown that cestodes accumulate substantial amounts of carbohydrates in reserve (Daugherty, 1956; Fairbairn et al., 1961; Markov, 1943; Read & Rothman, 1957b). It is generally accepted that these carbohydrates are predominantly stored as glycogen (Read, 1949; Reid, 1942). Lipids are vital for cestodes, acting as the primary form of concentrated energy storage. They also play an essential role in cellular structure and support various biochemical processes. Research has indicated that older proglottids, the segments of

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tapeworms, contain higher lipid concentrations (Brand & Van T., 1952). The current study focuses on the biochemical investigation of *Circumoncobothrium* sp., a cestode parasite found in *Mastacembalus armatus*.

2. Material And Methods

Sample collection- The worms were collected from the intestine of the freshwater fish *Mastacembelus armatus* and rinsed with distilled water. Following the wash, the worms were placed on blotting paper to remove excess moisture. They were then transferred to a watch glass and weighed using a sensitive balance. The worms were dried at a temperature of 50–60°C for 24 hours, and their dry weight was recorded.

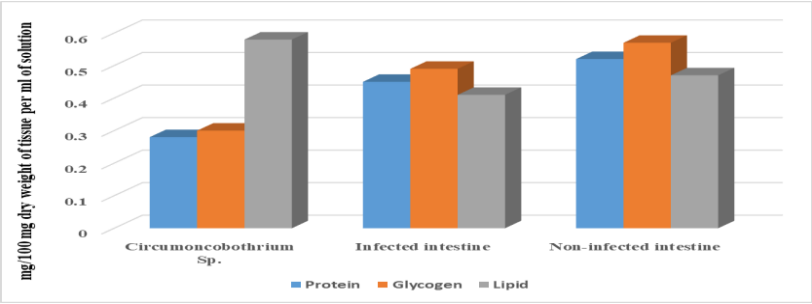
Biochemical estimation- The protein content in the cestode parasites was estimated using the Lowry method (1951). Glycogen content was determined using the method described by Kemp et al. (1954), and lipid content was assessed using the Folch method (1957).

3. Result And Discussion

Table no. 1:- Biochemical estimation of *Circumoncobothrium* Sp. species from Fresh water fish *Mastacembalus armatus*.

Name of Parameter	*Circumoncobothrium* Sp.	Host intestine	
		Infected	Non-infected
Protein (mg/100mg dry wt. of tissue per ml sol^{n})	0.28 ±0.016	0.45±0.021	0.52±0.022
Glycogen (mg/100mg dry wt. of tissue per ml sol^{n})	0.30±0.012	0.49±0.024	0.57±0.021
Lipid (mg/100mg dry wt. of tissue per ml sol^{n})	0.58±0.029	0.41±0.017	0.47±0.017

Graph No. 1:- Biochemical estimation of *Circumoncobothrium* Sp. species from Fresh water fish *Mastacembalus armatus*.



The biochemical analysis of *Circumoncobothrium* sp. and the host intestine (both infected and non-infected) revealed significant differences in protein, glycogen, and lipid content. *Circumoncobothrium*

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sp. showed lower levels of protein and glycogen compared to the host intestines, with the non-infected intestines having the highest concentrations of both proteins and glycogen.

Specifically, *Circumoncobothrium* sp. had a protein content of 0.28 ± 0.016 mg/100 mg dry weight of tissue per ml of solution. In comparison, the protein content in the infected and non-infected host intestines was 0.45 ± 0.021 mg/100 mg dry weight of tissue per ml of solution and 0.52 ± 0.022 mg/100 mg dry weight of tissue per ml of solution, respectively. Similarly, glycogen levels in *Circumoncobothrium* sp. were 0.30 ± 0.012 mg/100 mg dry weight of tissue per ml of solution, while the glycogen concentrations in the infected and non-infected host intestines were 0.49 ± 0.024 mg/100 mg dry weight of tissue per ml of solution and 0.57 ± 0.021 mg/100 mg dry weight of tissue per ml of solution, respectively.

In contrast, *Circumoncobothrium* sp. exhibited a higher lipid content of 0.58 ± 0.029 mg/100 mg dry weight of tissue per ml of solution, compared to the host intestines. The lipid levels in the infected and non-infected host intestines were 0.41 ± 0.017 mg/100 mg dry weight of tissue per ml of solution and 0.47 ± 0.017 mg/100 mg dry weight of tissue per ml of solution, respectively.

These findings indicate that while *Circumoncobothrium* sp. has lower protein and glycogen levels, it accumulates more lipids compared to the host intestines, with the non-infected host intestines generally showing higher levels of proteins and glycogen.

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Chemical Synthesis and Study of Physico-Chemical Properties of Magnetic Oxide Nanoparticles

Yogesh Gopal Mugale, V.S. Suryawanshi
Department Of Chemistry, SCSC OMERGA-413606, MAHARASHTRA, INDIA

Abstract

At the forefront of nanotechnology, magnetic oxide nanoparticles (MNPs) have exceptional potential for treating hyperthermia and delivering drugs precisely. Through the use of an alternating magnetic field, their special magnetic characteristics allow for precise targeting to certain biological locations, improving therapeutic efficacy. Multifunctional hybrid nanostructures that improve biocompatibility and expand the range of their therapeutic uses have been created as a consequence of the incorporation of MNPs into composite materials including liposomes and magnetic hydrogels. Magnetic nanoparticles may be used in a variety of biological settings by coating them to increase biocompatibility while maintaining their inherent magnetic properties. A range of chemical techniques are used in the manufacture of magnetic oxide nanoparticles, and each one provides exact control over the size, shape, and surface changes of the particles. To create MNPs with the right qualities for particular uses, processes including co-precipitation, sol-gel synthesis, and hydrothermal techniques are frequently used. The chemical production of magnetic oxide nanoparticles is examined in this work, along with their physico-chemical characteristics and possible uses in biomedicine. This study emphasises the importance of MNPs in nanomedicine and pinpoints future prospects for innovation and use in targeted treatments by analysing recent advancements in this quickly developing sector.

Keywords: Magnetic nanoparticles, Chemical synthesis, Physico-chemical properties, Biocompatibility, Drug delivery , Hyperthermia treatment ,Hybrid nanostructures

1. Introduction

Nanotechnology has had a profound impact on a wide range of scientific fields as a result of the unique characteristics and potential applications of the materials produced by this technology. There is a significant amount of importance placed on the structural characteristics and qualities of NMIOPs when it comes to determining their capabilities and applications. The magnetic properties of these materials, such as their saturation magnetization (MS), coercivity (HC), and remanence (MR.), are a significant area of research that is being conducted. Iron-based oxides such as magnetite (Fe_3O_4), hematite (Fe_2O_3), and maghemite (γ–Fe_2O_3) are examples of materials that exhibit superparamagnetic at dimensions that are less than 20 nanometres. In the absence of an external magnetic field, these nanoparticles do not display any magnetization, which makes them very useful for applications that need precise control of magnetic properties. [1–4]

MNPs possess a core and a coated shell, together forming the "typical" architecture of these particles. The core often consists of magnetic elements, including iron (Fe), nickel (Ni), and cobalt (Co), together with their related oxides. The coated shell regulates the interaction of the nanoparticles (NPs) with the medium, hence maintaining their structure and characteristics. MNPs possess a large surface area, facilitating surface changes, hence making them adaptable for many applications. The coating is essential for improving the biocompatibility of MNPs in biological applications while

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preserving their distinctive magnetic characteristics. Conversely, in the context of biological applications, the characterization of these nanostructures is paramount. Consequently, many approaches for assessing the chemical and physical characteristics of MNPs were devised.

Given that MNPs exhibit magnetic properties and confinement effects in all three dimensions, a wider array of unique qualities may be envisioned for practical medical applications and the investigation of basic scientific processes. They may also be used to examine fundamental scientific phenomena. [5]. The goal has been to facilitate the development of synthesis procedures that are not only straightforward but also economical. Chemical transformations are the most efficient means of controlling the size and shape of the object. To the contrary, it is possible to handle some limits that are associated with purity, dispersity, crystalline structure, and variable size by adjusting parameters such as composition and the processing solution. In order to avoid agglomeration and to ensure compatibility with biological systems, it is necessary to limit the size of the particles by careful execution and characterizations. A large amount of impact is exerted on the final features of the nanoparticles by the pH of the solution, the washing process, and the choice of washing solvent. The opposite is true; there is a dearth of comprehensive study on the relationship between pH, the washing solvent, and the eventual structure and features of nanoparticles. (6)–(8)

Applications of magnetic iron oxide nanoparticles in medicine

Magnetic iron oxide nanoparticles, which are often known as MIONs, are nanomaterials that are made of either maghemite (γ-Fe2O3) or magnetite (Fe3O4). Magnetic and superparamagnetic properties are shown by these particles, in addition to their small size, which ranges from one to one hundred nanometres in diameter. MIONs are used in a variety of biological systems, including the following:

- **Imaging contrast**

The presence of MIONs has the potential to enhance the pictures of tumours obtained by magnetic resonance imaging (MRI). Cells have been found to contain MNPs! Nanoparticles are created to allow the alignment of particles with each other under geomagnetic circumstances. This alignment is made possible by the nanoparticles. In addition, there is a substantial body of scientific literature that contains information on the use of fungi in the production of MNPs. The production of iron oxide nanoparticles, which has significant potential applications in the fields of biomedicine and cleaning, is carried out by a number of different fungal species. [9]

- **Drug delivery**

Through the use of MIONs, it is possible to facilitate the targeted delivery of therapeutic compounds to certain locations inside the body. MNPs have the potential to act as carriers for the delivery of drugs in a targeted manner due to their magnetic properties. Through the use of an external magnetic field, these characteristics make it possible to deliver specific substances to specific tissues. By using this method, the systemic effects of the drug are reduced, while at the same time, its bioavailability is improved, and focused distribution to the sick tissue is made easier, all in accordance with the specific needs associated with that tissue. It is possible for a pharmaceutical to improve therapeutic efficacy while simultaneously lowering the probability of experiencing adverse effects if it is given correctly.

- **Hyperthermia**

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The usage of elevated temperatures on tumours via MIONs may effectively eradicate the cellular composition of tumours. The elevated surface area-to-volume ratio of MNPs is one of its most notable benefits. This ratio allows extensive functionalization and modifications to meet certain biological needs. Adaptability facilitates the mixture of magnetic nanoparticles (MNPs) with specific belongings appropriate for many claims, with molecular detection, cancer therapy, and hyperthermia.

- **Molecular and cellular regulation**

MIONs has the capacity to regulate the cellular and molecular functions of the organism. Fluorescently tagged MNPs provide a diverse and efficient tool for visualising biological processes and structures at the molecular and cellular levels. Several preclinical investigations have shown that the use of MNPs in bioimaging has promise for illness diagnosis, monitoring disease progression, and evaluating therapy effectiveness [10].

The use of MIONs in clinical practices and biological research has been ongoing for an extended period. However, there are certain restrictions on their potential use, notably as:

- **Agglomeration**: It is possible for MIONs to cluster together; however this may be avoided by making surface alterations.

- **Size dependency**: The human body has the ability to eliminate MIONs that are either too big or too tiny.

- **Poor degradation**: MIONs may accumulate in normal tissues, potentially resulting in chronic inflammation. The preparation procedure used in the synthesis of MIONs may significantly affect their magnetic properties, surface chemistry, morphology, and dimensions.

Objectives Of The Study

1. To study on Magnetic iron oxide nanoparticles biomedical applications
2. To study on Chemical synthesis magnetic oxide nanoparticle

Chemical synthesis magnetic oxide nanoparticle

In the expansive and fast evolving domain of nanoparticle production, chemical techniques are mostly used. Chemical synthesis has been the predominant approach, accounting for over ninety percent of the published work to far. Furthermore, the coprecipitation process for creating iron salts is the most often used industrial method nowadays.[11–12]

1 Together with coprecipitation, precipitation

When it comes to the manufacture of magnetic nanoparticles (MNPs) containing magnetic metal oxide cores from suitable salt solutions, the two most common procedures that are used are precipitation and coprecipitation. It is possible to precisely modify the sizes of these MNPs as well as their magnetic properties thanks to the production processes that are simple, adaptable, and less hazardous.

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Metal ions are often used in situations where they are dissolved in a solvent, which results in the generation of a solution that is ideal for the synthesis of MNP. Examples of MNPs that may be created by these approaches include the synthesis of Fe3O4 or γ-Fe2O3 nanoparticles, which serves as an additional example. Following the conclusion of the reaction, a precipitate composed of Fe3O4 will be formed in the bottom of the reactor. Magnetic isolation and centrifugation are two other technologies that are beneficial for the recovery of environmental materials. The precipitate that is produced ought to have a pH that falls anywhere between 7.5 and 14. The synthesis of these particular forms of MNPs is very reliant on the sources of metal ions, in addition to the temperature, pH, and ionic strength of the medium in which the reaction takes place. Remember that this is an important factor to take into account [13]

The coprecipitation process is the most promising choice because to its user-friendliness and high output efficiency. Biomedicine applications often use it since it is user-friendly and requires less potentially dangerous materials and processes. The creation of iron oxide particles occurs via the ageing process, including the stoichiometric mixing of ferrous and ferric ions in an aqueous media. [14]. A chemical process that results in the creation of Fe3O4 may be expressed as follows:

$$Fe^{2+} + 2OH^- \rightarrow Fe(OH)_2$$

$$Fe^{3+} + 3OH^- \rightarrow Fe(OH)_3$$

$$Fe(OH)_2 + 2\,Fe(OH)_3 \rightarrow Fe_3O_4 + 4H_2O$$

After doing an analysis of the thermodynamics of this reaction, it is reasonable to anticipate that the entire precipitation of Fe3O4 will take place within a pH range of 9 to 14. This is because Fe3O4 is an unstable molecule that has the potential to undergo oxidation to γ-Fe2O3 when oxygen is present. The response might be communicated in the following manner:

$$Fe_3O_4 + 0.25O_2 + 4.5H_2O \rightarrow 3Fe(OH)_3$$

$$2Fe(OH)_3 \rightarrow \gamma\text{-}Fe_2O_3 + 3H_2O$$

To put a stop to this oxidation that is taking place in the atmosphere, it is necessary to establish an atmosphere that is devoid of oxygen. Through its movement through the solution, nitrogen is responsible for producing this state. The presence of nitrogen in the solution has the potential to lower particle size and impede oxidation. There are two distinct stages that may be distinguished within the process of coprecipitation. Following the formation of the first little nuclei in the medium, which occurs when the concentration of the species exceeds the critical supersaturation level, the crystal then begins to grow. The process is controlled by mass transport during the succeeding stage, which is the diffusion of solutes to the surface of the crystal. In order to successfully produce nanoparticles, it is necessary to differentiate between the two processes that are pertinent. Nucleation is not something that should take place throughout the period of crystal growth.

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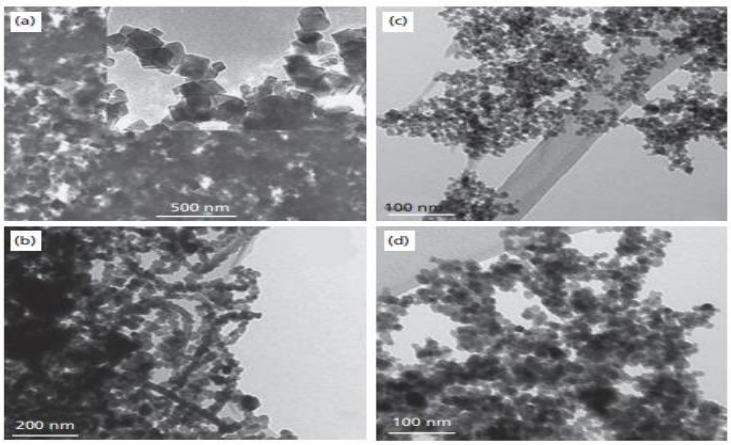

Figure 1. The following are examples of magnetite nanoparticle micrographs that were captured using a transmission electron microscope: (a) Sugimoto's method reaction with excess [OH]; (b) Sugimoto's method reaction without stirring and without excess [OH] or [Fe2+]; (c) Massart's method reaction with NH4 OH; and (d) Massart's method reaction with dispersing agent TMAOH and without NH4 OH.

2 Method of Thermal Decomposition

As a means of overcoming the limitations associated with the co-precipitation method, the thermal breakdown technique, which is sometimes referred to as pyrolysis, was developed. It was made easier to carry out this operation successfully by making use of non-aqueous solvents that had higher boiling points. The manufacture of highly crystalline MNPs of uniform sizes is made possible by this method. Decomposition of organometallic compounds in organic solvents is the first characteristic that distinguishes it from other types of reactions. Stabilising compounds, such as surfactants, enable this breakdown to take place at higher temperatures, which in turn facilitates the process. [15].

High-temperature decomposition of organic precursors

A diverse array of organometallic precursors for nanoparticles (NPs) exists, including acylketenes, N-nitroso phenylhydroxylamine, and carbonyls including different metallic centres such as Fe2+,3+, Mn2+,3+, Co2+,3+, and Ni2+,3+. Common stabilizing chemicals include hexadecyl amine, fatty acids, and oleic acids.

Decomposing iron precursors with heated organic surfactants enables the synthesis of iron oxide nanoparticles characterized by precise size control, a limited size distribution, and superior crystallinity. Furthermore, the generated particles are distributed across an extensive region. Besides Fe(Cup)3, Fe(CO)5, and Fe(acac)3, several more examples of iron precursors exist. Iron oleate may be synthesized by the decomposition of iron carbonyl at one hundred degrees Celsius in the presence of octyl ether and oleic acid. Subsequent to permitting the solution to reach room temperature, it is refluxed, and (CH3)3 NO is incrementally introduced. Magnetite nanoparticles with exceptional crystallinity and a size range of 4–16 nm may be produced by decomposing iron pentacarbonyl with oleic acid and then ageing the mixture at 300 degrees Celsius. The dimensions and morphology of the particles generated by this process are affected by various factors, including reaction duration,

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temperature, precursors, concentration, and the ratios of reactants to solvent. The surfactant's presence on particle surfaces aids in preserving the stability of the colloidal solution.

Particles measuring between 4 and 11 nanometres may develop due to the thermal degradation of iron oleate and iron pentacarbonyl in an organic solvent at varying temperatures. The iron oxide nanoparticles produced may dissolve in some organic solvents; however, the bulk remain insoluble in water. It is moreover a solvent. The particles in the report may range in size from 4 to 60 nm, contingent upon the duration of the reflux period. In a specific experiment investigating the breakdown of Fe(acac)3 in a high-temperature organic solvent, particles measuring 4, 6, 9, and 12 nm were generated. The particle size distribution is highly constrained, and they are encapsulated with 2,3-dimercaptosuccinic acid. Furthermore, these particles may be disseminated in water.

3 Hydrothermal Method

The hydrothermal process, which is sometimes referred to as the solvothermal method, is an example of a "bottom-up" synthesis methodology that may be used for IOMNP materials. In this method, the synthesis is carried out in an aqueous solution at a high temperature and pressure, and it is often carried out with the assistance of autoclaves or reactors. It is defined in the beginning by the fast nucleation and development of freshly synthesised MNPs, which ultimately leads to the creation of pure particles with morphologies that are tailored to the specific needs of the experiment. Micron nanoparticles (MNPs) are produced by a series of processes that take place during the hydrothermal process. These reactions include hydrolysis and oxidation. Several papers highlight the fact that the shape and crystallinity of the MNPs that are synthesised are dependent on the optimal mix of solvent, process time, pressure, and temperature. It is essential that minerals be soluble in water in order for the crystallization process to be successful.
In accordance with the reports, it is possible to produce magnetite nanoparticles by the use of hydrothermal techniques. The reactions that are carried out using these techniques take place in an aqueous medium that is contained inside reactors or autoclaves. Furthermore, the pressure must be greater than two thousand pounds per square inch, and the temperature must be higher than two hundred degrees Celsius. In the presence of hydrothermal conditions, the synthesis of ferrites takes place via two primary pathways: hydrolysis and the oxidation or neutralization of mixed metal hydroxides. These two reactions are quite much identical, with the exception of the fact that the first step involves the utilization of ferrous salts. The 24th In this method, the particles are subject to a significant amount of influence from the solvent, temperature, and the amount of time that has passed. The size of the particles that are produced as a consequence of the reaction is increased by both the length of time that the reaction is carried out and the amount of water that is present. The nucleation stage and the crystal development stage are the two steps that are involved in the production of particles. By increasing the temperature, the nucleation process is sped up in comparison to the creation of crystals, which ultimately results in a reduction in the size of the particles. As the duration of the reaction time increases, crystal development becomes more prevalent, which ultimately results in the formation of bigger particles. In order to produce magnetite nanoparticles with a diameter of 27 nanometres, the hydrothermal technique was used, and the sodium salt bis(2-ethylhexyl) sulfosuccinate was utilised as a surfactant.

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4 Polyol Method

When it comes to the synthesis of nanoparticles, the polyol approach is often considered to be among the most straightforward procedures. Through the use of this technique, the synthesis of nanoparticles from inorganic materials, such as alloys, sulphides, oxides, and fluorides, may be accomplished in a straightforward manner. The capability to generate high-crystalline hydrophilic MNPs in a single technique that is both cost-effective and readily scalable is one of the most significant advantages.

5 Sol–Gel Method

The sol–gel method is a wet chemistry approach. This method employs metal alkoxide hydrolysis and polycondensation processes to generate a gel at ambient temperature. Dissolving metallic salts in water or other solvents produces a sol or colloidal solution that is uniformly distributed throughout the medium. Van der Waals forces are formed between the particles inside the system. Elevating the temperature and agitating the mixture both enhance the extent of particle-to-particle contact. Upon heating the combination until the solvent evaporates, the solution will eventually desiccate and transform into a gel.

The sol-gel technique is a wet-chemical method reliant on the hydrolysis and condensation of precursors inside a colloidal solution. This is the foundation of the procedure. individual A metal oxide network (gel) is generated due to a chemical reaction or the removal of a solvent. Acidic catalysis yields a polymeric gel, while basic catalysis produces a colloidal gel. The rates of condensation and hydrolysis are critical process parameters that significantly affect the characteristics of the resulting particles.

A slower and more regulated hydrolysis rate may provide smaller particles. Moreover, temperature, pH, concentration, and the particular solvent influence particle size. Heating the gel to 400 degrees Celsius produces γ-Fe2O3 particles measuring between 6 and 15 nanometres. Considering the experimental circumstances, the technique allows the precise prediction of particle structures in advance. This method allows the encapsulation of γ-Fe2 O3 nanoparticles inside a transparent, inorganic silica matrix that withstands temperature variations.[16] The majority of approaches for synthesising iron oxide-silica composites need an initial step involving the amalgamation of iron oxide and silica precursors in a solvent to generate a sol. Conversely, the sol-gel process yields more reactive iron oxide-silica aerogel composites compared to the traditional iron oxide technique.

6 Microemulsion Method

A microemulsion consists of three components: an amphiphilic surfactant, water, and oil, forming a thermodynamically stable dispersion. This method involves integrating precursor materials throughout many stages of the microemulsion process to generate nanoparticles (NP). Nanoparticles are generated as a result of chemical processes occurring inside microemulsion droplets, which are distinguished by their close closeness to one other.

Within the framework of water-in-oil microemulsion systems, the microdroplets that are present in the aqueous phase are distributed over the whole of the petroleum phase. In order to protect

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the microdroplets, surfactant molecules protect them. As a result of the presence of surfactant molecules, the particles are unable to nucleate, mature, or aggregate appropriately. Microdroplets that are composed of water will integrate iron salt into the microemulsion in the event that an iron salt solution is put into the microemulsion. By continuing to collide with one another, these little droplets will eventually combine and break apart. In the event that two reactants are injected into a microemulsion, the result will be the formation of a precipitate. The two processes that support the creation of particles are the aggregation of nuclei and the interchange of particles between droplets. There is no doubt that the precipitate can be eliminated from the surfactants via the process of separation.

Iron oxide nanoparticles with a remarkably uniform size distribution were produced as a result of the integration of an aqueous core containing aerosol-OT/n-hexane reverse micelles into a microemulsion. Through the use of the aqueous core, the reactants are dissolved. An aqueous core that included a solution of Fe3+ and Fe2+ salts in a ratio of 4:1 was one of the individual components that comprised this report. The precipitation process is carried out with the assistance of a sodium hydroxide solution that has been deoxygenated.

Magnetite nanoparticles were produced as a result of the introduction of nitrogen gas, which resulted in the reduction of their dimensions and the creation of a more uniform size distribution (Figure 5). At lower temperatures, the nanoparticles were created using the synthesis process. Because of the minuscule size of the aqueous core, which is measured in the nanometre range, the particles that are produced are generally less than 15 nanometres and have an extraordinarily narrow size distribution. The capacity of microemulsion technology to control the size of particles by adjusting the diameters of the aqueous core is one of the most significant advantages of this technology.

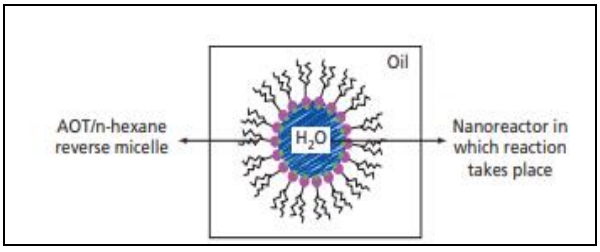

Figure 2. Structure of an aqueous core with aerosol-OT/n-hexane reverse micelles.

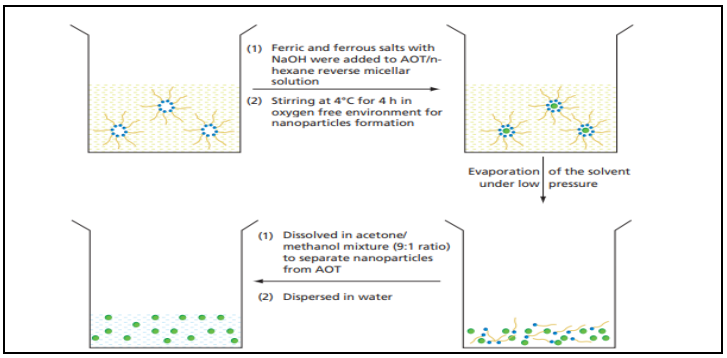

Figure 3. Highly monodispersed iron oxide nanoparticles are produced using the microemulsion technique.

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7 Pyrolysis Methods

It is well knowledge that spray pyrolysis is a technique that is used in the production of a wide variety of materials, one of which is magnetic nanoparticles (MNPs). The use of this method includes the production of very minute droplets of precursor solutions, which are subsequently aerosolised into an environment that is heated to a reasonable degree. Following the evaporation of the solvent, the remaining solute is collected on a substrate, and it is then subjected to a series of chemical reactions in order to produce the compound that is required.

The synthesis of iron oxide nanoparticles may also be accomplished by the use of sonolysis, which is the process of degrading organometallic precursors. When structural hosts, polymers, or organic capping agents are present, it is possible that they will hinder the formation of particles. The rapid collapse of holes that are formed by acoustic waves results in the production of a zone with a high temperature, which makes it easier for ferrous salts to be converted into magnetic nanoparticles. The sonolysis of an aqueous solution of Fe(CO)5, in combination with sodium dodecyl sulphate, has the potential to produce a hydrosol that contains amorphous magnetite nanoparticles. Through the use of sonolysis, it has been possible to successfully produce superparamagnetic iron oxide nanoparticles that have been accurately characterised. In the course of this inquiry, the particles that have been created are coated with oleic acid, which is a surfactant. This coating prepares the particles for dispersion in a solution of chitosan. This is carried out in order to make the investigation easier. An excellent level of stability is shown by the 65 nm coated particles. Particularly important for a number of applications are the magnetic properties, the diameters of the particles, the size distribution, the particle shape, and the size distribution. It is possible to create a wide variety of particle qualities via the use of a variety of production techniques, and these characteristics may be obtained through a variety of different approaches. The aerosol/vapor method, polyol methods, and electrochemical approaches are some other ways that may be used for deposition.

8 Non-Thermal Methods

The synthesis of MNPs may be accomplished via the use of non-thermal procedures, which are methods that do not need the use of high temperatures during the production process. In order to avoid issues with aggregation or thermal breakdown, these approaches are often used since they have the potential to produce nanoparticles (NPs) that possess unique characteristics.

Common non-thermal methods used for MNP synthesis are:

- **Chemical Reduction**

By reducing metal ions with chemical agents, it is possible to produce magnetic nanoparticles without the need for increased temperatures. This can be accomplished without the need for increasing the temperature. This method is not only simple and cost-effective, but it can also be used to a wide variety of metals. In addition to this, it is often used in the production of metal nanoparticles, which may include those that are made of platinum, silver, and gold.

- **Electrochemical Synthesis**

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Electrochemical reactions occur at the electrodes, producing MNPs as a consequence. This technology may be used to achieve simplicity, the ability to scale up, and control over size and form. It's also critical to note that it works well with a variety of materials, including conducting polymers, metals, and metal oxides.

- **Microwave-Assisted Synthesis**

Through the use of microwave radiation, reaction mixtures are heated, which enables the heating process to be both rapid and uniform. When compared to conventional methods of heating, this strategy consumes less energy, results in higher yields, and has reaction rates that are far faster [17]

- **Ultrasound-Assisted Synthesis**

The application of ultrasonic waves to a reaction mixture results in the formation of acoustic cavitation, which prompts the synthesis of particles more often. Better homogeneity, control over particle size, and rapid reaction times are all benefits that come with using this technology.

Physical and chemical properties of magnetic oxide nanoparticles

Magnetic oxide nanoparticles have many physical and chemical properties, including:

- **Magnetism**

A physical property that can be observed by how an object reacts to a magnet.

- **A high ratio of surface area to volume**

A unique property of magnetic nanoparticles that is different from their bulk materials.

- **Size-related magnetism**

A distinctive characteristic of magnetic nanoparticles that differentiates them from their bulk counterparts

- **Colloidal stability**

Magnetic nanoparticles have higher colloidal stability because they don't magnetically agglomerate.

- **Chemical stability**

Magnetic nanoparticles have higher chemical stability, which is important for biomedical applications.

- **Narrow size distribution**

Magnetic nanoparticles have a narrow size distribution, It is crucial for biological applications.

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- **Zeta potential**

A physical characteristic of colloidal dispersions, including nanoparticle suspensions. It is the potential difference between the bulk solution and the static fluid layer adhered to the dispersed particle.
Other properties of magnetic oxide nanoparticles include:

- **X-ray diffraction**: Utilised for the purpose of analysing the arrangement of atoms inside the magnetic core, which provides information on the crystalline structure of the atoms.
- **Thermal decomposition**: A widely accepted method for synthesizing high-quality magnetic nanoparticles.
- **Microwave synthesis**: Can be used to generate metal oxides in the nanoscale range.

Conclusion

The modern techniques that are used to manufacture iron oxide nanoparticles make it possible to customise the surface for a variety of applications, one of which is the production of superparamagnetic particles that have an extremely narrow size distribution. The capacity of magnetic nanoparticles to be effectively targeted to specific regions inside the body by means of an alternating magnetic field is one of the many advantages that they provide. Other advantages include its use in treatments such as hyperthermia. These two advantages are only two of the innumerable advantages that magnetic nanoparticles provide. Magnetic nanoparticles are excellent for drug administration because they give large replacement levels. This is because to the raised surface-area-to-volume ratio that can be achieved with these particles. The incorporation of these nanostructures into composites, such as magnetic hydrogels or liposomes, results in the formation of new classes of multifunctional hybrid nanostructures. In addition to exhibiting improved biocompatibility, these nanostructures have the potential to be used in a wider range of therapeutic applications. The continual presence of a number of problems that need solutions is shown by these systems. Magnetic nanoparticles (MNPs) have a significant impact on their effectiveness due to the size and shape of these particles. As a consequence of this, it is of the utmost importance to develop appropriate synthetic procedures and conduct further research in order to ascertain the optimal performance of the final materials. The aggregation of MNPs is another cause for concern since it has the potential to reduce the effectiveness of these particles and to pose toxicity issues. The fact that iron oxide nanoparticles are often considered to be less hazardous than a great number of other types of nanoparticles is something that should be taken into consideration, despite the fact that toxicity studies are required. The applications of particles have a considerable impact on the magnetic properties of those particles, and the size of the particles has a substantial impact on the magnetic properties of those particles. For applications, the techniques that are used to produce particles are very important. In the field of biomedicine, magnetic nanoparticles have the potential to enhance diagnostic procedures and treatment choices, ultimately leading to an improvement in the quality of life of individuals.

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Phytochemical analysis of aerial part of *Justicia repens* using different solvent

Kiran B. Patil[1], Madhuri S.Patil[2]

[1] *Department of Science and Humanities, KCES COEM, Jalgaon-425001, Maharashtra,*
[2] *Department of Chemistry, J.D.M.V.P. Samaj's, Shri. S. S. Patil Art's, Shri. Bhausaheb T. T. Salunkhe Commerce and Shri. G. R. Pandit Science College, Jalgaon-425001, Maharashtra, ,*
E-mail: madhurisatishpatil@gmail.com, kbpatilsnk@gmail.com

Abstract: The plant extract of *Justicia repens* has been of significant interest for decades, with various parts such as stems, flowers, leaves, bark, seeds, and tumors being used for extraction with different solvents. The main objective of this analysis was to investigate the phytochemical constituents and functional groups in methanolic, ethanol, acetone, chloroform, and ethyl acetate extracts from the plant's aerial parts. Initial screening through Fourier Transform Infrared (FT-IR) spectroscopy identified the presence of secondary metabolites, including alkaloids, flavonoids, tannins, terpenoids, phenols, and phytosterols. FT-IR analysis also identified functional groups including alkanes, hydrocarbons, carboxylic acids, esters, and alcohols.

Keywords: FT-IR, phytochemical, *justicia repens*, Medicinal plant.

1. Introduction:

Plants containing built in active ingredients to cure disease and relive from different pains. Plant incorporates many various phytochemicals having ability to anti insecticide and anti fungicide [1] Specific plant species applicable for various ailment on humans. Traditionally, herbal extracts were known to be effective against microorganisms as a result, plants form the basis of modern medicine. Plants produce phytochemicals to protect themselves but recent studies indicates that many phytochemicals can also protect humans against infection diseases [2]. The FT IR spectrum is identifying the functional group of the plant extract based on peak value ratio.

Justicia repens is a pharmacologically important plant belongs to Acanthaceae family. Plant species abundant in Gujarat, Maharashtra, Karnataka, Kerala, Tamilnadu, and dried region in India, and Srilanka. *Justicia repens* is commonly found in nature in areas such as waste fields, along rivers, and beside railway lines [3]. *Justicia repens* is a small bush plant having height 10-30cm has multiple branches short spikes at nodes up to 3-5cm tiny blue flowers about 2-3mm leaves are 3-5cm [4]. The plant part is dries using to cure human temp of body it is applied with oil to cure fungoid septicity [5].

FT-IR study gives functional group having with methanolic, ethanol, acetone, chloroform, and ethyl acetate extracts of *Justicia repens* aerial part, which help to grip against different disease.

2. Materials and methods

Plant collection and authentication

Healthy, young aerial part of *Justicia repens* collected for analysis from Jalgaon District, Maharashtra, India authentication from botanical department of Nutan Maratha College, Jalgaon

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Preparation of plant extract

By the maceration process 250 g of dried crude grinded aerial part of sample immersed in 700 ml of ethanol, methanol, chloroform, ethyl acetate and acetone for 7 days. Respective extract was shifted individually using whatsmann No. 41 filter paper The extract were carried in vacuum at 60 ^{0}C using rotary evaporator, with the extract held at 4 ^{0}C in cooling condition.

Phytochemical analysis

The extract of aerial part of *Justicia repens* were screening (Table-1) phytochemicals by standard methods [6] Flavanoids, Total Phenolics and Tannins, Terpenoids were exams by the method [7] Saponins were analyzed by the method [8].

FT-IR spectroscopy analysis

The FT-IR analysis was conducted using the Perkin Elmer spectrometer system [9]. The plant extract was first centrifuged at 3000 rpm for 10 minutes and then filtered through Whatman No. 1 filter paper using a high-pressure vacuum pump [10]. The test sample was analyzed with the same solvent using a Perkin Elmer spectrophotometer within the wavelength range of 400–4000 nm, and the peaks were identified and their corresponding values recorded.

Result and discussion

Preliminary phytochemical characterization

Table 1

Qualitative phytochemical screening of different extract of aerial part of *Justicia repens*.

Sr. No.	Phytochemicals	Different Solvents				
		Methanol	Ethanol	Acetone	Chloroform	Ethyl acetate
1	Tannins	+	+	+	+	-
2	Terpenoids	+	+	-	+	-
3	Flavonoid	+	+	+	-	-
4	Phenol	+	+	+	-	-
5	Phytosterol	-	+	-	-	+
6	Saponins	+	+	-	-	-

FT-IR spectroscopy analysis

FT-IR spectroscopic analysis is an effective technique for identifying various chemical bonds and phytochemical functional groups based on infrared absorption values. The aerial part extract of *Justicia repens* was examined using FT-IR, which facilitated the classification of different bimolecular compound groups. The FT-IR spectrum revealed prominent peaks ranging from 630 to 3315 cm^{-1}, each corresponding to specific functional groups within the sample. The spectra exhibited notable overlap of absorption peaks from various components [11].

Methanolic extract

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Alcohols and phenolics in aerial part extract (Fig.1) (O-H stretching) showed a peak at 3315.63cm^{-1} while carboxylic acid (O-H stretching) showed a peak at 3288.70 cm^{-1} alkanes (O-H stretching) shows peak at 2927.94 and 2864.29 cm^{-1}. Amines and Amides (N-H stretching) showed peak at2353.16cm^{-1}. While carbonyl (C=O stretching) shows at 1724.36cm^{-1} and Amide (C=O stretching) shows peak at 1645.28cm^{-1}. The peak of Aromatic hydrocarbons (C=C stretching) shows at 1444.68 cm^{-1} and 1417.80 cm^{-1}. Acids (C-O stretching) showed peak at1251.80 cm^{-1}. The peak for ethers (C-O stretching) was observed at 1053.13cm^{-1}. In methanolic aerial part extract *Justicia repens* alkyl halides were observed at the peak of 630.72 cm^{-1} [12].

Chloroform extract

FT-IR peaks (Fig.2) shows (O-H stretching) at 3379.29cm^{-1}. The aliphatic (C-H stretching) at peak 2924.09cm^{-1}.While (C-O stretching) of carboxylic at 2351.23 cm^{-1}.the aldehyde (C= stretching) shows at peak at 1730.15 cm^{-1}. At peak 1450.47cm^{-1}. Shows (C-H stretching) alkane. The peak for alkane (C-H stretching) shows at 1379.10 cm^{-1}. At 1247.94 cm^{-1} shows (C-O stretching) alcohols.1041.56 cm^{-1} peak value shows vinyl ether (C-O stretching). The 719.45 cm^{-1} and 576.72 cm^{-1} peak shows alkyl halide of chloride and iodide respectively [13].

Ethyl acetate extract

The aerial stock extract of *Justicia repens* shows FT-IT peaks (Fig.3) at 3427.15 cm^{-1},3367.71 $cm^{-1,}$3317.56 cm^{-1} shows alcoholic (O-H stretching) Aliphatic primary amine (O-H stretching). The peak at 2924.09 cm^{-1}, 2856.58 cm^{-1} shows (C-H stretching) peak of alkane. At 1732.08 cm^{-1}, 1656.85 cm^{-1} shows (C=O stretching) at 1456.26 cm^{-1} and 1384.89 cm^{-1}. The peak at 1255.66 cm^{-1} shows (C-O stretching) Acids Peak at 1039.63 cm^{-1} (C-O stretching) shows vinyl ether . At 989.48 cm^{-1} peak value shows (C-N stretching) amine. While alkyl halide (C-Cl stretching) shows peak at 723.31 cm^{-1} [14].

Acetone extract

The plant extract (Fig.4) with acetone shows a peak at 3367.71cm^{-1},3352.28 cm^{-1} (O-H stretching) to aliphatic functional group. The alkane peak shows at (C-H stretching) 2926.01 cm^{-1}, 2862.36 cm^{-1}. At peak 2684.91 cm^{-1}shows (C-H stretching) towards alkanes. While aldehyde (C=O starching) shows peak 1730.16 cm^{-1}. alkane peak shows at 1450.47 cm^{-1},1379.10 cm^{-1} (C-H stretching). Acids shows peak at (C-O stretching) 1249.87cm^{-1}. Ether shows at 1174.68 cm^{-1} (C-O-C stretching). Vinyl ether shows (C-O streching) peak at 1037.70 cm^{-1}. At 977.91 cm^{-1} shows aromatic compound (C-H bending) Alkane shows peak (C-H bending) at 914.91cm^{-1}. At peak 721.26 cm^{-1},597.08 cm^{-1} 514.99 cm^{-1} shows alkyl halides of (C-Cl, I, Br stretching) chlorine , Iodide , bromine respectively [15].

Ethanolic extract

The extract of *Justicia repens* aerial part shows FT-IR peaks (Fig.5). Alcohol (O-H stretching) shows at peak 3329.14 cm^{-1}.3282.84 cm^{-1}. The aromatic shows peak at 3120.82 cm^{-1} (C-H stretching) .While hydrocarbon shows at (C-H Stretching) 2927.94 cm^{-1}. Alkane shows peak (C-H stretching) at 2862.36 cm^{-1}. Acids shows (C=O stretching) at 1726.29 cm^{-1}. At 1392.61 cm^{-1} shows (C-F stretching) towards alkyl halide. Acid shows (C=o stretching) at 1263.37 cm^{-1}. The ether shows (C-O stretching) peak at1051.20 cm^{-1}. Alkene shows (-C-H stretching) peak at 921.97 cm^{-1} and 705.95 cm^{-1}. Alkyl halide shows peak (C-I, C-Br stretching) at 596 cm^{-1} and 526.57 cm^{-1} [15] .

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The infrared functional group characteristics identified in the test sample align with those reported in the literature. Recent findings suggest the presence of various functional groups, indicating that the sample may be a promising candidate for a range of pharmaceutical applications.

FT-IR peaks values and functional groups of different aerial part extract of *justicia repens*.

Sr. No.	Bond/ Stretching	Freq (cm^{-1})	Functional group (Methanolic extract)
1	O-H Stretch	3315	Alcohols/Phenols
2	O-H Stretch	3288	Carboxylic Acid
3	C-H Stretch	2927	Alkane
4	C-H Stretch	2864	Alkane
5	N-H Stretch	2353	Amine/amide
6	C=O Stretch	1724	Carbonyl group
7	C=O Stretch	1645	Amide
8	C=C Stretch	1444	Aromatic
9	C=C Stretch	1417	Aromatic hydrocarbon
10	C-O Stretch	1251	Acids
11	C-O Stretch	1053	Ethers
12	C-Cl Stretch	630	Alkyl halides

	Bond/ Stretching	Freq (cm^{-1})	Functional group (Chloroform extract)
1	O-H Stretch	3379	Alcohols
2	C-H Stretch	2924	Aliphatic
3	C=O Stretch	2351	Carbonyl group
4	C=O Stretch	1730	Aldehyde
5	C-H Stretch	1450	Alkane
6	C-H bending	1379	Alkane
7	C-O Stretch	1247	Acids
8	C-O Stretch	1047	Vinyl ether
9	C-Cl Stretch	719	Alkyl halides
10	C-I Stretch	576	Alkyl halides

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Table 4

Sr. No.	Bond/ Stretching	Freq (cm^{-1})	Functional group (Acetone extract)
1	O-H Stretch	3367	Aliphatic
2		3352	
3	C-H Stretch	2926	Alkane
4		2862	
5		2684	
6	C=O Stretch	1730	Aldehyde
7	C-H Stretch	1450	
8	C-H bending	1379	Alkane
9	C-O Stretch	1249	Alkane
10	C-O-C Stretch	1174	Carboxylic acid
11	C-O Stretch	1037	Vinyl Ether
12	C-N	977	Amine
13	C-H Stretch	914	Alkene
14	C-Cl Stretch	721	Alkyl halides
15	C-I Stretch	594	
16	C-Br Stretch	514	

Table 5

Sr. No.	Bond/ Stretching		Freq (cm^{-1})	Functional group (Ethyl acetate extract)
1	N-H		3427	Amine/amide
2	O-H Stretch		3344	Aliphatic primary amine
3			3300	
4	C-H Stretch		2924	Alkane
5			2856	
6	C=O Stretch		1732	Aldehyde
7			1656	
8	C-H Stretch		1456	Alkane
9	C-H Stretch		1384	Alkane
10	C-O Stretch		1255	Acids
11	C-O Stretch		1039	Vinyl Ether
12	C-N		989	Amine
13	C-Cl Stretch		723	Alkyl halides

Table 6

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Sr. No.	Bond/ Stretching	Freq (cm^{-1})	Functional group (Ethanolic extract)
1	O-H Stretch	3329	Alcohols/Phenols
2		3382	
3	C-H Stretch	3120	Aromatic hydrocarbon
4		2927	
5	C-H Stretch	2862	Alkane
6	C=O Stretch	1726	Acids
7	C-F Stretch	1392	Alkyl halides
8	C=C Stretch	1263	Acids
9	C-O Stretch	1051	Ether
10	C- H Stretch	921	Alkene
11		705	
12	C-I Stretch	596	Alkyl halides
13	C-Br Stretch	526	

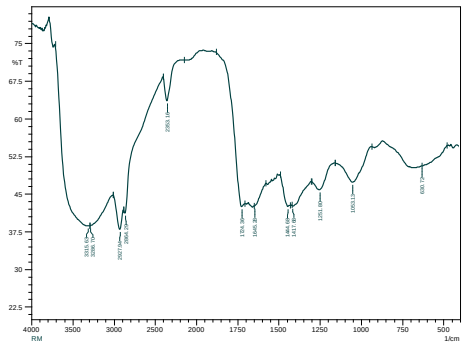

Fig. 1. FT-IR chromatogram of methanolic extract of aerial part of *Justicia repens*.

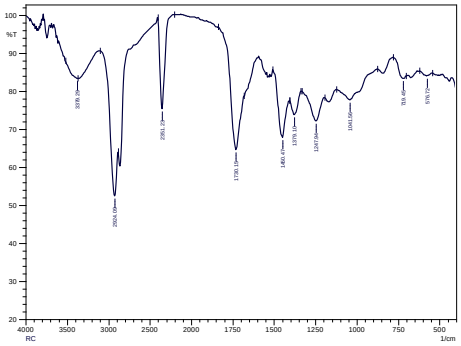

Fig. 2. FT-IR chromatogram of Chloroform extract of aerial part of *Justicia repens*.

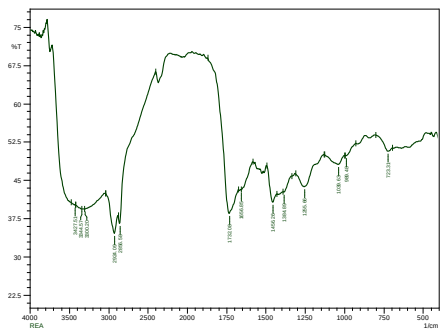

Fig.3. FT-IR chromatogram of Ethyl acetate

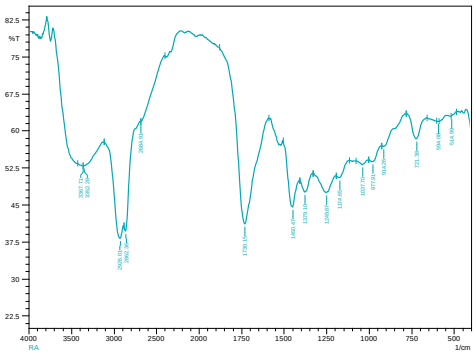

Fig.4. FT-IR chromatogram of Acetone

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extract of aerial part of *Justicia repens*. extract of aerial part of *Justicia repens*.

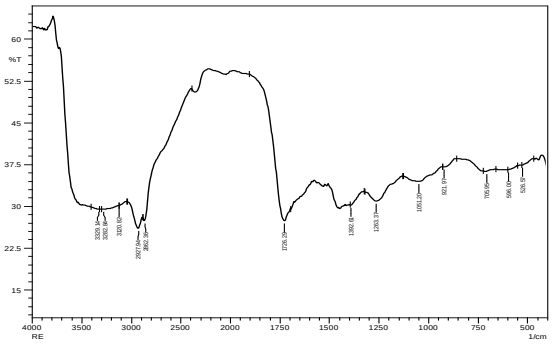

Fig.5. FT-IR chromatogram of Ethanolic extract of aerial part of *Justicia repens*.

Conclusions

Justicia repens is a highly regarded restorative herb with notable medicinal properties. FT-IR (Fourier Transform Infrared) analysis of its aerial parts reveals a diverse range of functional groups and an abundance of phytochemicals. These compounds are linked to various biological activities, supporting the plant's traditional use in ethnomedicine. The findings suggest that the phytochemical components of *Justicia repens* could have valuable applications in medicinal treatments.

Acknowledgement

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Conflicts of interest

The authors declare no conflict of interest.

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Synthesis, Characterization and Antibacterial / Antioxidant Investigation of Metal-Salen Schiff Base Metal Complexe.

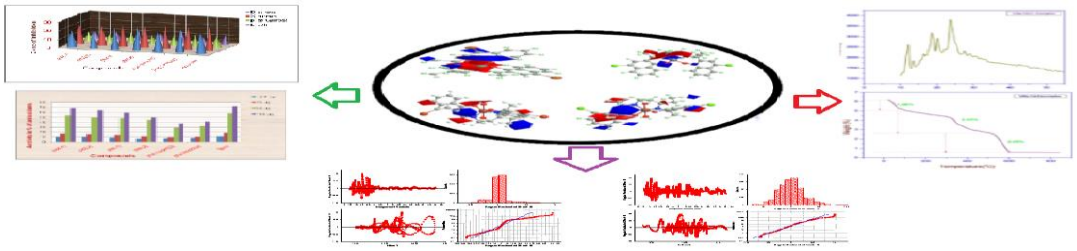
Bhagwat T. Vhanale[1*], Avinash T. Shinde[1], Dhananjay V. Bondar[2], Nagesh J. Deshmukh[3]
[1*] *P.G. Department of Chemistry, S.C.S.College, Omerga, (Maharashtra), India- 413606.*
[1] *P.G. Department of Chemistry, N.E.S. Science College, Nanded, (Maharashtra), India- 431605.*
[2] *P.G. Department of Chemistry, S.C.S.College, Omerga, (Maharashtra), India- 413606.*
[3] *P.G. Department of Chemistry, N.E.S. Science College, Nanded, (Maharashtra), India- 431605.*
E-mail: bvhanale777@gmail.com

Abstract:

Four novel synthesized Ni(II) and Fe(III) complexes of have been characterized by UV vis., FT-IR, ^{1}H & ^{13}C NMR, LC-MS, TGA-DTA, ESR and powder X-ray diffraction data to elucidate there structures. The IR results confirmed the tetradentate binding of the ligand involving two napthol oxygen and two azomethine nitrogen. ^{1}H NMR & ^{13}C NMR spectral data of the (H_2L2) and its metal complexes agreed well with proposed structures. Thermo gravimetric Studies for Ni(II) and Fe(III) complexes indicated the presence of coordinated water molecules and final product is the formation of metal oxide. From the powder X-ray diffraction data it could be finding that Ni(II) complexes are having triclinic while Fe(III) complexes are monoclinic system with space group P1. The ESR lines showed that, Ni(II) complexes are diamagnetic in nature and Fe(III) complexes are having five unpaired electrons. In order to evaluation of antibacterial activity of Schiff base ligand and its metal complexes were screened by using two Gram-positive and two Gram-negative bacterial strains, the newly synthesized metal complexes are showed more potent than the Schiff base ligand. Furthermore, the antioxidant activity were determined by the reduction of 1,1-diphenyl-2-picryl hydrazyl (DPPH). The Schiff base ligands are exhibited better antioxidant activity than its metal complexes.

Keywords: Tetradentate Schiff bases; Ni(II) and Fe(III) complexes; PXRD; TGA-DTA; ESR; antibacterial activity; antioxidant activity.

Graphical Abstract:



1. Introduction

Transition metal complexes with Schiff bases are specific area for research to inorganic chemist due to their wide range of various biological activities [1-3]. Also, The interest of research is developing because they can prepare easily in high % yield under normal reaction conditions as well as they are having a broad range of complexion behavior [4,5].The chemical, structural and spectral

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properties of metal complexes are often strongly dependant on the nature of the ligand structure. In the recent years, in medicinal department the metal bases drugs have gained much importance. They are used for the treatment of tumor [6], cancer [7], anti-inflammatory [8] disease. Also, some of Schiff bases and their metal complexes have been exhibited various bioactivities like antibacterial [9-10] antioxidant [9-10] antifungal [11-12], Brine shrimp lethality [12], DNA damage assays [12]. As like various bioactivities some of Schiff base metal complexes show versatile applications and characteristics properties like catalytic activity [13], alkaline phosphatase inhibition [14], insulin mimetic properties [14], physicochemical properties [15], and magnetic properties [16], phenoxazinone synthase activity [17], photochromic [18] and enzymatic activity [19].

The N2O2 O-hydroxy aromatic compounds are the important moiety of Schiff bases have attracted considerable attention because of their interesting physicochemical properties and pharmacological activities. This type of Schiff base metal complexes finds applications in other fields, such as homogeneous catalysis [20], Catalytic oxidation [20], emission behaviour [21], redox property [21-22], fluorescent chemosensor for detection of Fe^{2+} ions [23], potentiometric sensor [24], catalytic used in Heck [25] & Suzuki reaction [25] Dyes [26], Polymers [26], Phenoxazinone synthase mimicking activity [27], Catalase mimic activity [28].

It was reported that the DFT calculations of Ni(II) complexes is the ligand acts as a tetradentate Schiff base and coordinated to Ni(II) via two Nitrogen imine and two Oxygen phenolic atoms such complexes show a distorted square planar geometry [29,30] around the central metal ion and Fe(III) complexes show octahedral geometry [31] with high spin (*d5*) state [32-33]. Also, Ni(II) and Fe(III) complexes with electron-withdrawing groups improve nonlinear optical properties [34-35]. Also the Ni(II) and Fe(III) ion complexes with tetradentate donor Schiff base gives excellent antibacterial [36-39] and antioxidant activities [36-39]. Therefore, it has been initiate interesting to study the metal complexes with N_2O_2 O-hydroxy aromatic Schiff bases. On the other hand, Schiff bases derived from 2-hydroxy-1-napthanone have been comprehensively studied because they form stable complexes with metal ions due to the presence of a phenolic –OH group and presence of azomethine group at their ortho- position.

Recently we have reported here the synthesis of Ni(II) and Fe(III) complexes of Schiff bases containing halogenated N2O2 O-hydroxy aromatic moiety derived from pentane-1,3-diamine with 1-(4-bromo-1-hydroxynaphthalen-2-yl)ethanone and 1-(4-chloro-1-hydroxynaphthalen-2-yl)ethanone and characterized by various physicochemical techniques and studied their antibacterial and antioxidant activities. The result of this article will be very useful to the upcoming researchers to gain more information about the antibacterial and antioxidant activities of Ni(II) and Fe(III) complexes of halogenated N2O2 donor Schiff bases.

2. Experimental

2.1 Materials

All the reagents and required chemicals were purchased commercially from AURA, SPECTROCHEM & TCI chemical company. All solvents were purchased of gradient Grade and used without purification. The metal salts, $Ni(OAC)_2.4H_2O$ was purchased from Fine-Chem Ltd., and $Fe_3O(OAC)_6.3H_2O$ was purchased from Sigma Aldrich. *In vitro* antibacterial activity was screened by using Mueller Hinton Agar (MHA) obtained from Hi media (Mumbai).

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2.2 Analytical methods

In the laboratory, the purity of the product was checked by thin-layer chromatography (TLC). It was carried out on 0.25-mm E Merck gel plates (60F-254) and spots were visualized by UV light. Melting points of the newly synthesized compounds were determined by using the digital apparatus Koefler Banc and are uncorrected. The elemental analysis (C, H, and N) was carried out by using Perkin-Elmer 240 elemental analyzer. The UV- Visible spectrophotometer was recorded on a UV-1800 series spectrophotometer in chloroform. The FT-IR spectra were recorded as KBr pellets on diffuse reflectance attachment (Miracle Attenuated Total Reflectance Attachment) covering the range 4000-600 cm^{-1} with an Agilent FT-IR spectrophotometer. 1H and 13C NMR spectra of ligand and its Ni(II) and Fe(III) complexes were recorded in DMSO-*d6* with Bruker Avance III HD 300 operating at 300 MHz at 21^{o}C using TMS as an internal standard. ESI-MS has recorded on LC-MS (ESI) mass spectrometer at 70 eV. ESR analysis was performed the instrument ESR-JEOL, JEsS-FA200 ESR spectrometer with X band (8.75-9.65 GHz) at room temperature, XRD was measured on instrument X-ray diffractometer, Ultima IV, Rigaku corporation, and TGA-DTA with Detector Type DTG-60H.

2.2.1 Synthesis of ligands (H_2L1) and (H_2L2)

Synthesis of Schiff base ligand (H_2L1) is reported in the previous article [40**].** The 1:2 molar mixture of pentane-1,3-diamine (10 mmol) and 1-(4-chloro-1-hydroxynaphthalen-2-yl)ethanone (20 mmol) in absolute ethanol (25mL) was refluxed with a catalytic amount of glacial acetic acid (2-3 drops) for about 2-3 h. For better results, the reaction mixture was rest overnight. The needle-shaped pale yellow product (H_2L2) was filtered off, washed with hot water, and recrystallized with absolute ethanol.

2.2.2 [E]2,2'-((pentane-1,3-diylbis(azanylylidene))bis(ethan-1-yl-1-ylidene))bis(4-chloronaphthalen-1-ol) (H_2L2)

Yield- 406.52 mg, 80 %, Color- yellow, M.P. 192 – 194 $^{\circ}$C.

FT-IR(KBr,cm^{-1}): 3399(νOH),1640(νC=N),1525(νC=C),1072(νC−N−C),875,765(νC−Cl).

*^{1}HNMR($CDCl_3$)(ppm)δ:*14.09(s,Ar−OH,2H),8.50-6.79(m,10H,Ar−H),4.09(t,J=4.5Hz,−CH_2,2H),3.65(m,J=4.6Hz,−CH,1H),2.46(s,−CH_3,3H),2.35(s, −CH_3,3H),2.33(q,J=4.3Hz,−CH_2,2H),1.81(m,J=4.1Hz,−CH_2,2H), 1.04(t, J=4.1Hz,−CH_3,3H).

*^{13}CNMR($CDCl_3$)(ppm)δ:*175.50(−C=N−),170.95(C−O),137.45-106.66(Ar−C−),136.21(−C−Cl),54.22(−N−C−H),41.71(−N−CH_2−),34.76(HC−C−CH_2−),29.56(H_3C−C−CH−),14.57(−N=C−CH_3),10.24(−C−CH_2−CH−).

ESIMS (m/z): 508.15 (63.9 %).

2.3 General procedure for synthesis of metal complexes.

The methanolic solution of Schiff base ligand (H_2L1) and (H_2L2) (10mmol) was added to a hot methanolic solution of respective metal acetate (10mmol). The resulting solution was refluxed for 5-7 h. the reaction mixture was cooled to room temperature and immediate separation of a small amount of side product was filtered off. After evaporation of the filtrate were obtained a product.

2.3.1. Synthesis of [Ni(L1)] and [Ni(L2)] complexes

[Ni(L1)]-(1E,1'E)-N,N'-(pentane-1,3-diyl)bis(1-(4-bromo-1-(l1-oxidanyl)naphthalen-2-yl)ethan-1-imine)nickel(II)

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Molecular Formula: [$C_{29}H_{26}Br_2N_2NiO_2$] , Molecular Weight: 653, Yield- 406.52 mg, 80 %, Color− yellow, M.P. 192 – 194 °C.

FT-IR(KBr,cm^{-1}):

1597(νC=N), 1520(νC=C),1020(νC−N−C),879,788(νC−Br),578(νM−O),491(νM−N).

*^{1}HNMR(CDCl$_3$)(ppm)δ:*8.53-6.80(m,10H,Ar−H),4.11(t,J=4.5Hz,−CH_2,2H),3.70(m,J=4.6Hz,−CH,1H),2.46(s,−CH_3,3H),2.36(s,−CH_3,3H),2.23(q,J=4.3Hz,−CH_2,2H),1.82(m,J=4.1Hz,−CH_2,2H), 1.05(t, J=4.1Hz,−CH_3,3H).

*^{13}CNMR(CDCl$_3$)(ppm)δ:*174.81(−C=N−),170.52(C−O),134.14-108.36(Ar−C−),134.09(−C−Br),54.36(−N−C−H),41.83(−N−CH_2−),34.37(HC−C−CH_2−),29.36(H_3C−C−CH−),14.49(−N=C−CH_3),10.23(−C−CH_2−CH−).

m/z: 651.97 (100.0%).

Elemental Analysis: C, 53.34; H, 4.01; Br, 24.47; N, 4.29; Ni, 8.99; O, 4.90

[Ni(L2)]- (1E,1'E)-N,N'-(pentane-1,3-diyl)bis(1-(4-chloro-1-(l1-oxidanyl)naphthalen-2-yl)ethan-1-imine), nickel(II)

Molecular Formula: [$C_{29}H_{26}Cl_2N_2NiO_2$], Molecular Weight: 564,

FT-IR(KBr,cm^{-1}):

1590 (νC=N),1527(νC=C),1027(νC−N−C),863,790(νC−Cl),566(νM−O),485(νM−N).

*^{1}HNMR(CDCl$_3$)(ppm)δ:*8.50-6.78(m,10H,Ar−H),4.10(t,J=4.5Hz,−CH_2,2H),3.72(m,J=4.6Hz,−CH,1H),2.48(s,−CH_3,3H),2.35(s,−CH_3,3H),2.25(q,J=4.3Hz,−CH_2,2H),1.85(m,J=4.1Hz,−CH_2,2H),1.05(t,J=4.1Hz,−CH_3,3H).

*^{13}CNMR(CDCl$_3$)(ppm)δ:*175.55(−C=N−),171.34(C−O),137.37-108.50(Ar−C−),137.20(−C−Cl),54.09(−N−C−H),41.77(−N−CH_2−),34.51(HC−C−CH_2−),29.39(H_3C−C−CH−),14.39(−N=C−CH_3),10.28(−C−CH_2−CH−).

m/z: 562.07 (100.0%)

Elemental Analysis: C, 61.74; H, 4.65; Cl, 12.57; N, 4.97; Ni, 10.40; O, 5.67

2.3.2. Synthesis of [FeL1(H_2O)$_2$] and [FeL2(H_2O)$_2$] complexes

[FeL1(H_2O)$_2$]-(1E,1'E)-N,N'-(pentane-1,3-diyl)bis(1-(4-bromo-1-(l1-oxidanyl)naphthalen-2-yl)ethan-1-imine)iron(III) dehydrate

Molecular Formula: [$C_{29}H_{30}Br_2FeN_2O_4$]

Molecular Weight: 686.22

FT-IR(KBr,cm^{-1}):

1587(νC=N), 1531(νC=C),1022(νC−N−C),889,788(νC−Br),588(νM−O),480(νM−N).

*^{1}HNMR(CDCl$_3$)(ppm)δ:*8.53−6.80(m,10H,Ar−H),4.12(t,J=4.5Hz,−CH_2,2H),3.71(m,J=4.6Hz,−CH,1H),2.47(s,−CH_3,3H),2.35(s,−CH_3,3H),2.21(q,J=4.3Hz,−CH_2,2H),1.81(m,J=4.1Hz,−CH_2,2H), 1.04(t, J=4.1Hz, −CH_3,3H).

*^{13}CNMR(CDCl$_3$)(ppm)δ:*174.80(−C=N−),170.50(C−O),134.12−108.32(Ar−C−),134.10(−C−Br),54.364(−N−C−H),41.82(−N−CH_2−),34.35(HC−C−CH_2−),29.37(H_3C−C−CH−),14.47(−N=C−CH_3),10.22(−C−CH_2−CH−).

m/z: 685.99 ((100.0%)

Elemental Analysis: C, 50.76; H, 4.41; Br, 23.29; Fe, 8.14; N, 4.08; O, 9.33.

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[FeL2(H_2O)$_2$]-(1E,1'E)-N,N'-(pentane-1,3-diyl)bis(1-(4-chloro-1-(l1-oxidanyl)naphthalen-2-yl)ethan-1-imine)iron(III)dihydrate

Molecular Formula: [$C_{29}H_{30}Cl_2FeN_2O_4$], Molecular Weight: 597.31

FT-IR(KBr,cm^{-1}):

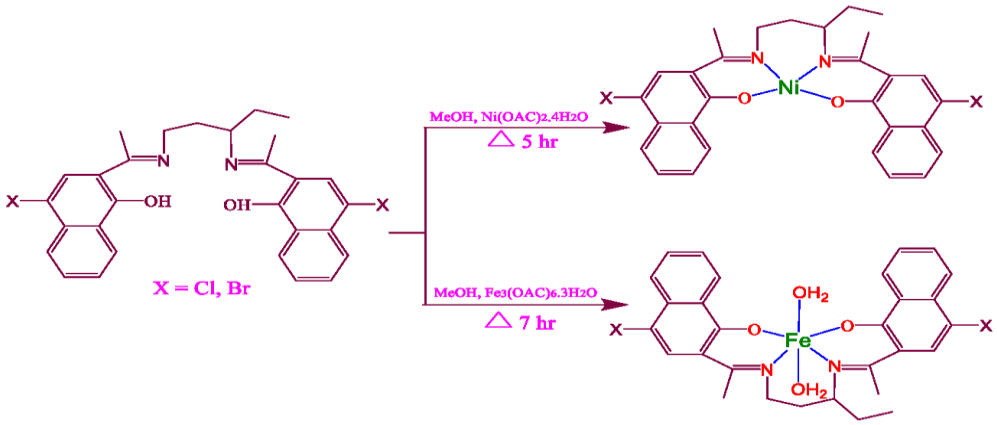
1585(νC=N),1525(νC=C),1022(νC−N−C),875,790(νC−Cl),567(νM−O),485(νM−N).

*^{1}HNMR($CDCl_3$)(ppm)δ:*8.50−6.78(m,10H,Ar−H),4.12(t,J=4.5Hz,−CH_2,2H),3.78(m,J=4.6Hz,−CH,1H),2.44(s,−CH_3,3H),2.33(s,−CH_3,3H),2.21(q,J=4.3Hz,−CH_2,2H),1.83(m,J=4.1Hz,−CH_2,2H),1.00(t,J=4.1Hz,−CH_3,3H).

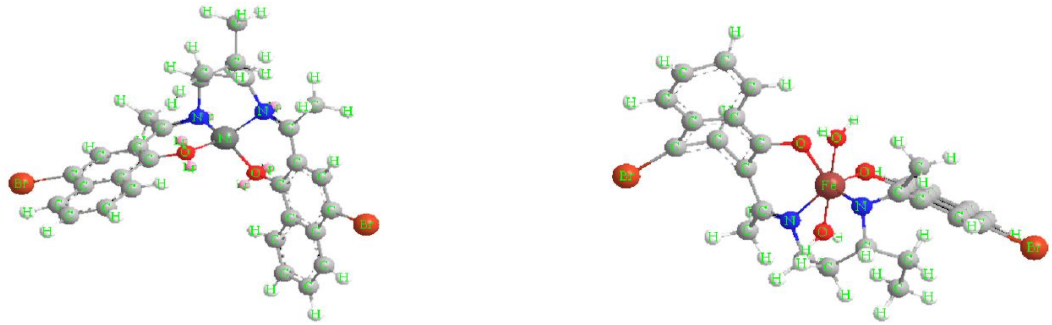
*^{13}CNMR($CDCl_3$)(ppm)δ:*175.54(−C=N−),171.33(C−O),137.35−108.52(Ar−C−),137.22(−C−Cl),54.10(−N−C−H),41.75(−N−CH_2−),34.52(HC−C−CH_2−),29.40(H_3C−C−CH−),14.40(−N=C−CH_3),10.29(−C−CH_2−CH−).

m/z: 596.09 (100.0%)

Elemental Analysis: C, 58.31; H, 5.06; Cl, 11.87; Fe, 9.35; N, 4.69; O, 10.71



Scheme1. Synthesis of metal complexes.



(a) Ni(II) complexes (b) Fe(III) complexes

Figure 1. Optimized view of metal complexes.

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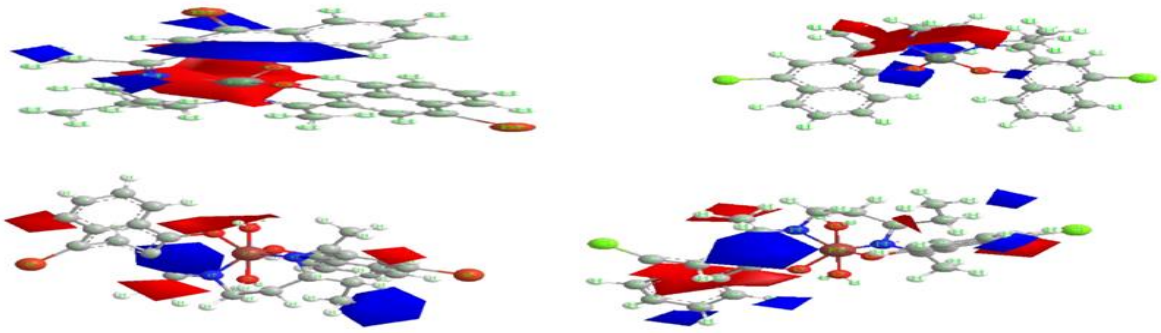

Figure 2. The Molecular orbital surfaces of metal complexes.

2.4 Evaluation of antibacterial

2.4.1 Antibacterial activity

Antibacterial assay of newly synthesized Schiff bases and its metal complexes were screened *in vitro* against different species of bacteria, *Bacillus licheniformis*, *Bacillus species*, *Escherichia coli*, and *Staphylococcus aureus* by using a well diffusion method. Mueller-Hinton agar (MHA) medium is used for Microbial Suspension (100 *ul*) containing 108 CFU ml^{-1} of bacteria. The extracts were diluted in 100% dimethyl Sulphoxide at the concentrations of 5mg/ml. The Mueller Hinton agar was melted and cooled to 48-50 ^{o}C and standardized inoculums (1.5 X 108 CFU/ml, 0.5McFarland) were added aseptically to the molten agar and pours into sterile Petri dishes to yield a solid plate. By using the Well diffusion method the product was prepared in the seeded Agar plate. Incubation of the plates is done in the incubator overnight at 37 ^{o}C. The antibacterial spectrum of the extract had determined for the bacterial species in terms of zone sizes around each well. The diameters of the zone of inhibition were produced by the compound were compared to standard Ampicillin.

2.4.2 Antioxidant activity

The antioxidant activity of synthesized Schiff base ligands (H_2L1 &H_2L2) and their metal complexes were determined by using the DPPH method. The antioxidant activity of these compounds was carried out at different concentrations (12.5, 25, 50, and 100 μg). Different concentrations of test compounds and standard butylated hydroxyanisole (BHA) were taken in separate test tubes and by adding distilled water each test tube was adjusted to 100 μL. Hydroxyl radical scavenging activities were determined by the earlier reported method [41]. The percentage scavenging of DPPH free radical for each concentration of test compounds was calculated concerning an absorbance of control using the formula given below.

$$\% \text{ scavenging activity} = \frac{[\text{Control optical density} - \text{Sample optical density}]}{\text{Control optical density}} \times 100$$

3. Results and discussion

3.1 UV- visible Spectra

The UV spectra of Schiff bases were studied in the polar solvent while complexes are in DMF solvent. The absorption band of Schiff bases in range 350–384 nm due to n→ π* transition of the C=N imine group. Also, the complexes are given the same absorption in this region with very low intense bands above 490 nm due to metal ligand bonding of metal complexes.

3.2 FT-IR Spectra

FT-IR analysis of the synthesized complexes help in getting on how is the ligand coordinated to the metal ion. The IR frequencies of ligands and respected metal complexes are depicted in table 1. In the IR spectrum of the ligand (H_2L2), absorption bands due to phenolic–OH, azomethine (−C=N), and phenolic ν(C−O) group have appeared at 3399 cm^{-1}, 1590 cm^{-1} and 1322 cm^{-1} respectively. The IR

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spectra of all the complexes, it was observed that the absence of absorption band due to phenolic –OH group at 3399 cm^{-1} of ligand indicates the formation of bond between metal ion and phenolic oxygen atom. This is further confirmed by the change in absorption frequency of phenolic ν(C−O) which are shown in the region 1275–1277 cm^{-1} indicating the coordination to metal ion *via* oxygen atom of phenolic group. The absorption frequency of azomethine ν(−C=N) function shifted to lower frequency and appeared in the region 1520–1531 cm^{-1}. This is confirmed that the involvement of nitrogen atom of azomethine group in complexation with metal ion.

The formation of metal–ligand bonding was further confirmed by the appearance of low intense bands in the region 564−575cm^{-1} and 462−491cm^{-1} which assigned to frequencies of ν(M−O) and ν(M−N) stretching bands are appear in region respectively.

Table 1. IR frequencies of Schiff base ligands and respected metal complexes.

Compound	ν(OH)	ν(H2O)	ν(C-O)	ν(C=N-)	ν(M-O)	ν(M-N)
H_2L1	3485	--	1320	1592	--	--
H_2L2	3399	--	1322	1597	--	--
[Ni(L1)]	--	3425	1275	1520	570	491
[Ni(L2)]	--	3428	1277	1527	568	490
$[FeL1(H_2O)_2]$	--	3417	1275	1531	575	485
$[FeL2(H_2O)_2]$	--	3430	1277	1525	564	462

3.3 NMR Spectroscopy

The ^1H NMR spectra of Schiff base ligand and its metal complexes were recorded in $CDCl_3$. The ^1H NMR spectra of the ligand H_2L2 displayed singlet at 14.09 ppm due to the proton of phenolic –OH. The siglets appeared at 2.46 ppm and 2.35 ppm due to 6H of two $-CH_3$ groups. The signals due to aromatic protons have resonated as multiplets in the region at 6.80−8.68 ppm. The most significant evidence for the formation of bonding of phenolic oxygen atom to metal ion *via* deportation is the disappearance of phenolic –OH group signal at 14.09 ppm. When compared to the ^1H NMR spectra of ligand and its metal complexes, all the signals due to protons have been shifted towords down field δ value confirming the complexation of metal ion with the ligand.

The ^{13}C NMR spectrum of ligand H_2L2 displayed signals at δ 175.5 ppm due to azomethine carbon. The appearance of signals at δ 170.70 ppm and 135.01 ppm due to carbon-bearing oxygen and the carbon bearing to halogen atom respectively. When compared to the ^{13}C NMR spectra of Schiff base ligand to its metal complexes, the signals due to azomethine carbon and carbon-bearing oxygen have been shifted towords down field δ value confirming the complexation of metal ion with the ligand.

3.4 LC-MS

The ESI mass spectrum of the Schiff base ligand and their metal complexes are given their structure confirmation. The Schiff base ligand **(H_2L1)** and **(H_2L2)** appearance of molecular ion peak at m/z 437 and m/z 409 respectively which is equivalent to its molecular weight. Similarly, the ESI mass spectrum respected metal complexes are given an appropriate molecular ion peak concerning their molecular weight. The [NiL1], [NiL2], $[FeL1(H_2O)_2]$ and $[FeL2(H_2O)_2]$ are showed a molecular ion peak recorded at m/z 651.97, m/z 562.07, m/z 596.09 and m/z 685.99 respectively.

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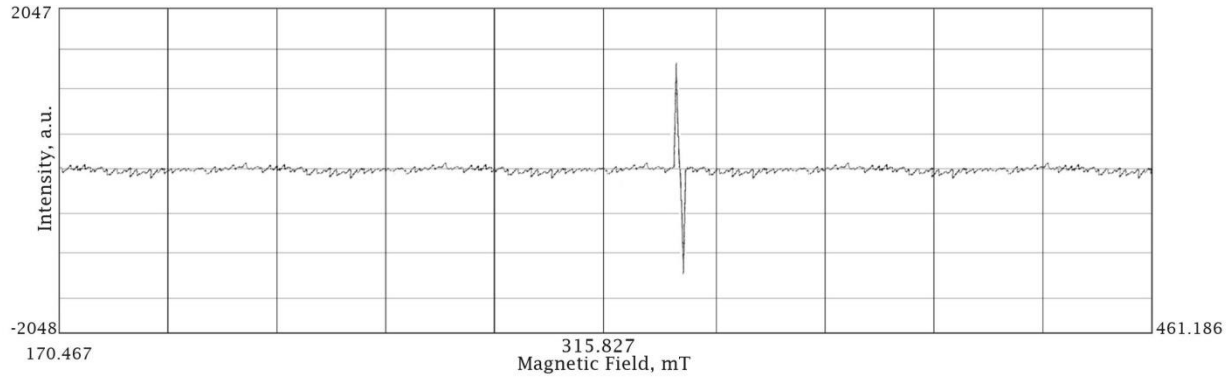
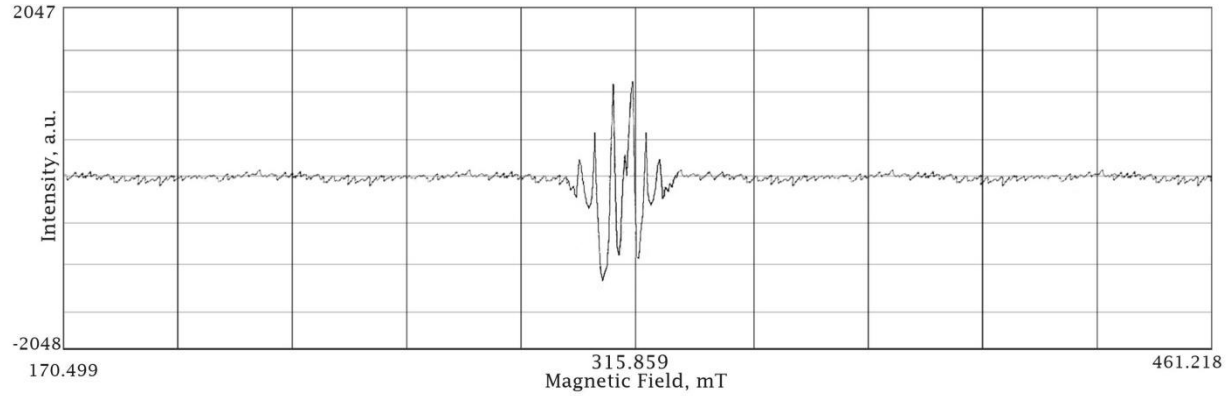
3.5 ESR

The ESR spectrum of [NiL1] and [FeL2(H_2O)$_2$] complexes provides information about the geometry and nature of the ligating sites of the Schiff base and metal. The EPR spectrum was recorded in DMSO at room temperature and specta are shown in figure 3. Complex [NiL1] displayed well resolved an isotropic behavior with sharp single and without any hyperfine splitting having 2.0797, indicative of square planar Ni(II) geometry. The EPR spectrum of complex [FeL2(H_2O)$_2$] exhibits six well defined anisotropic signals with hyperfine splitting which may attributed to five unpaired electron interaction of Fe(III) with nuclear spin I = 5/2.



a) [NiL1] complex



b) [FeL1(H_2O)$_2$] complex

Figure 3.ESR of synthesized metal complexes

3.6 Single crystal X-ray diffraction

The newly synthesized metal complexes were soluble in organic solvents like DMSO and DMF, for single crystal studies crystals are not obtained. The values of bond length and bond angle were done by using chem3D (ChemOffice) software; they are tabulated in table 4 and 5 respectively. In order to test the crystallinity of presented metal complexes, we used powder XRD pattern of Ni(II) and Fe(III) complexes. Under the powder X-ray diffraction pattern of synthesized metal complexes were scanned in the range 0-80° (θ) at 1.54 Å wavelength. From figure 5 it is seen that, the pattern of the curves decreases from maximum to minimum intensity indicating the synthesized metal complexes are in amorphous nature. From XRD data, table 2 shown Ni(II) complexes were

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crystallized with triclinic system while Fe(III) complexes are in the monoclinic system having space group P1. The calculated lattice parameters for Ni(II) complexes is ($a \neq b \neq c$) a = 9.1524, b = 13.6320, c =17.2330 with $\alpha \neq \beta \neq \gamma$ and for Fe(III) complexes is a = 7.0696, b = 14.8954, c = 05.3504 with $\alpha = \beta \neq \gamma$.

The definite diffraction data of Ni(II) and Fe(III) complexes, like angle (2θ), inter-planar spacing (d-value), FWHM, Crystallite size, dislocation density, and micro strain are summarized in table 3.the maximum diffraction pattern of NiL1, NiL1, [FeL1(H_2O)$_2$] and [FeL2(H_2O)$_2$] complexes exhibited at 2θ [d value (Å)] = 23.91 (3.71), 30.87 (2.89), 34.80 (2.57) and 45.84 (1.97), respectively. The particle size was calculated by applying Debye-Scherer's formula:

$$D = 0.9\,\lambda/\beta.\cos\theta$$

Where, λ is the wavelength of radiation, β is full width with half maximum (FWHM) of attribute peaks and θ is the diffraction angle.

Also, the various parameters like Crystallite size,(L), dislocation density (ρ) and micro strain (ε) were calculated for synthesized Ni(II) and Fe(III) complexes as shown in table 3 using the following equations:

$$L = K\,\lambda/b.\cos\theta$$
$$\rho = 1/L^2$$
$$\varepsilon = b.\cos\theta/4$$

Figure 5 shows different types of graph viz., Residual versus fitted graph, Skewed graph and Quantile - Quantile graph were obtained by using XRD data as well as OriginPro-2018. Graphically examining plots of residuals are Gaussian distributed i.e. normally distributed have constant variance and more residuals close to zero. In Quantile – Quantile graph, the graph line is oriented out off the straight line. It indicates the relationship between the X variable (2θ) and the average Y (intensity) is non-linear.

Table 2. PXRD data of metal complexes.

Complex	**[NiL1]**	**[NiL2]**	**[FeL1(H_2O)$_2$]**	**[FeL2(H_2O)$_2$]**
Empirical Formula	[$C_{29}H_{26}Br_2N_2NiO_2$]	[$C_{29}H_{26}Cl_2N_2NiO_2$]	[$C_{29}H_{30}Br_2N_2FeO_4$]	[$C_{29}H_{30}Cl_2N_2FeO_4$]
Formula weight	653	564	686	597
Temperature	298	298	298	298
Crystal System	Triclinic	Triclinic	Monoclinic	Monoclinic
Space Group	P1	P1	P1	P1
a (Å)	9.1524	9.1524	7.0696	7.0696
b (Å)	13.6320	13.6320	14.8954	14.8954
c (Å)	17.2330	17.2330	05.3504	05.3504
α (°)	77	77	90	90
β (°)	76	76	90	90
γ (°)	89	89	78	78
Z	4	4	4	4

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Volume, $Å^3$	2043.36	2037.18	561.36	551.10

Table 3. Multiple peaks fit for metal complexes.

Compound	No. of peaks	2θ	d-spacing (Å)	FWHM β	Crystallite size D(mm)	Dislocation density,nm^{-2} (δ x10^{-3})	Micro strain (εx10^{-3})
NiL1	1	12.00	7.36	1.03	07.6940	16.8925	43.0916
	2	13.58	6.51	0.68	11.6349	07.3869	25.1862
	3	18.77	4.72	1.00	07.9749	15.7231	26.6410
	4	20.19	4.39	0.78	10.2505	09.5171	19.2849
	5	23.91	3.71	1.05	07.5330	17.6220	21.7298
NiL2	1	12.73	6.94	0.47	16.8003	03.5429	18.5988
	2	18.47	4.79	0.89	09.0031	12.3369	23.9857
	3	24.36	3.65	1.72	04.7136	45.0080	34.8471
	4	25.89	3.43	0.86	09.1373	11.9773	16.5016
	5	27.98	3.18	0.44	18.5370	02.9101	07.73316
	6	30.87	2.89	0.95	08.5995	13.5223	15.1414
FeL1	1	22.30	3.98	0.48	16.6550	03.6050	10.7608
	2	25.43	3.49	1.74	04.6541	46.1656	33.8259
	3	28.62	3.11	1.58	05.0219	39.6504	27.0584
	4	31.98	2.79	0.83	09.8877	10.2283	12.7256
	5	33.85	2.64	0.72	11.4833	07.5834	10.3676
	6	34.80	2.57	1.54	05.3851	34.4830	21.5215
FeL2	1	10.84	8.15	0.46	17.0785	03.4284	21.4875
	2	12.48	7.08	0.48	16.3683	03.7324	19.4730
	3	23.04	3.85	1.51	05.3550	34.8715	32.4066
	4	26.73	3.33	1.19	06.8069	21.5821	22.0246
	5	45.84	1.97	1.09	07.9038	16.0072	11.2610

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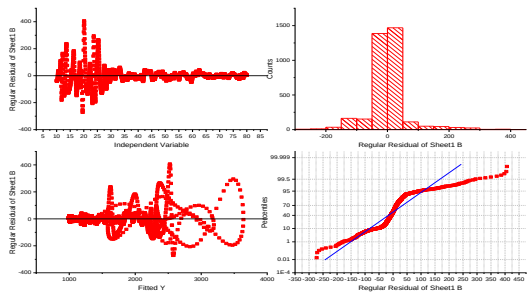
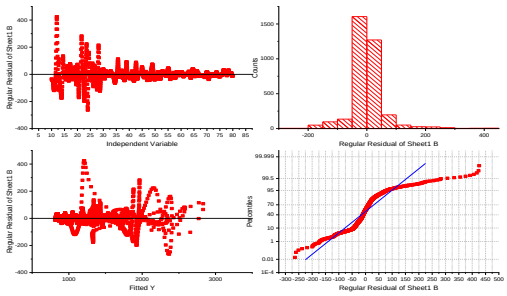
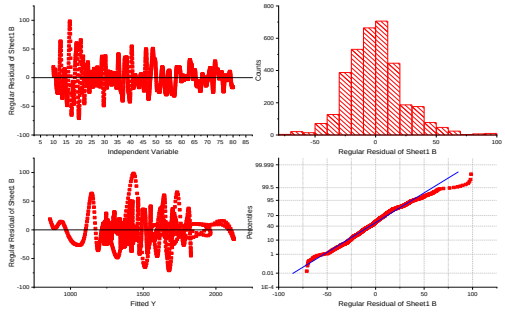


(a) NiL1

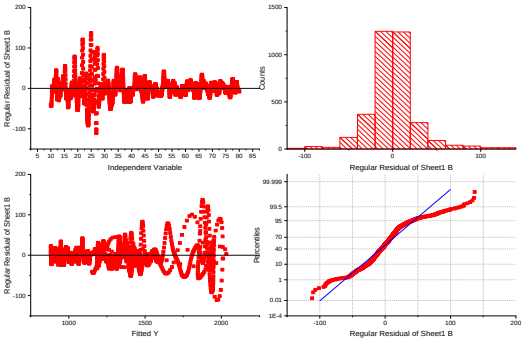


(b) NiL2

(b)



(c) FeL1(H_2O)



(d) FeL2(H_2O)

Figure 4.Graphical representation of Residual fits of metal complexes

Table 5. Selected bond angles (°) for metal complexes.

Bond angle type	[FeL1(H_2O)$_2$]	[FeL2(H_2O)$_2$]	Bond angle type	[NiL1]	[NiL2]
O(37)-Fe(36)-O(38)	78.38	78.16	N(15)-Ni(36)-N(19)	95.05	95. 03
O(37)-Fe(36)-O(32)	77.52	77.61	N(15)-Ni(36)-O(32)	91.86	91.57
O(37)-Fe(36)-O(11)	82.66	82.52	N(15)-Ni(36)-O(11)	172.82	172.21
O(37)-Fe(36)-N(15)	126.9	126.86	N(19)-Ni(36)-O(32)	172.84	172.45
O(37)-Fe(36)- N(19)	136.01	136.66	N(19)-Ni(36)-O(11)	91.83	91.73
O(38)-Fe(36)-O(32)	127.52	127.11	O(32)-Ni(36)-O(11)	81.17	81.58
O(38)-Fe(36)-O(11)	79.81	79.22	--	--	--
O(38)-Fe(36)- N(15)	147.75	147.28	--	--	--
O(38)-Fe(36)- N(19)	84.14	84.41	--	--	--
O(32)-Fe(36)-O(11)	140.76	140.72	--	--	--
O(32)-Fe(36)- N(15)	81.52	81.86	--	--	--
O(32)-Fe(36)- N(19)	82.03	82.12	--	--	--
O(11)-Fe(36)- N(15)	83.96	83.26	--	--	--
O(11)-Fe(36)- N(19)	133.31	133.33	--	--	--
N(15)-Fe(36)- N(19)	87.11	87. 10	--	--	--

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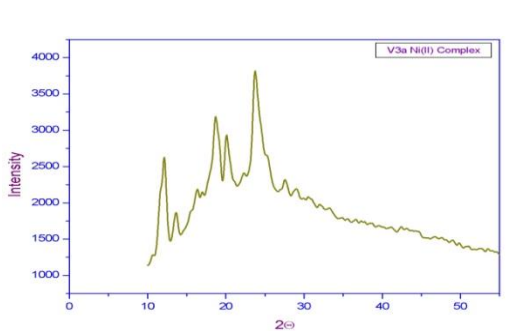
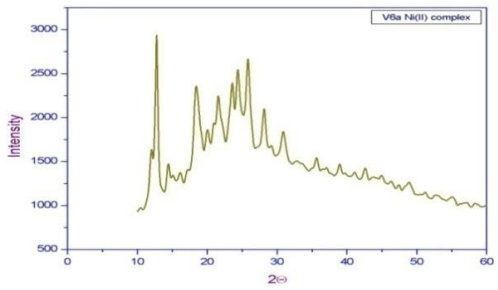
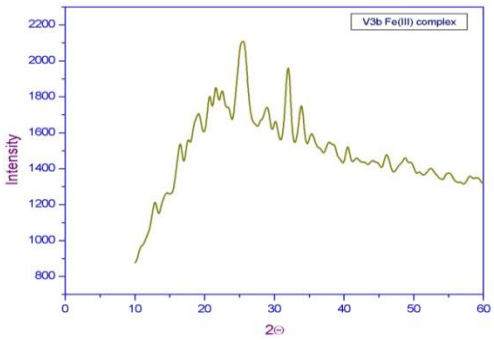


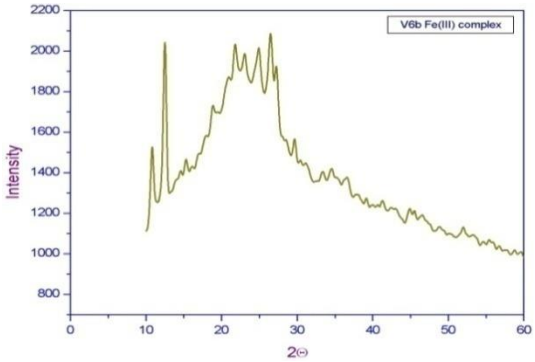
(a) NiL1 complex



(b) NiL2 complex



(c) $[FeL1(H_2O)_2]$ complex



(d) $[FeL1(H_2O)_2]$ complex

Figure 5. Graphical representation of XRD data of synthesized metal complexes.

3.7 TGA-DTA

In order to study the thermal stability of the metal complexes, thermogravimetric (TG) and differential thermal analyses (TGA) were carried out for newly synthesized Ni(II) and Fe(III) complexes. TGA/DTA curves of Ni(II) and Fe(III) complexes show different peaks of decomposition. In Ni(II) complexes, the first step of degradation occurred in the range 62 – 99 ^oC, due to the loss of non-coordinated water molecules with a practical weight loose of 1.06%. In second and third step of degradation occurred in the range of 100 – 600 ^oC, due to the removal of the ligand part from the metal atom with a practical weight looses2.43% and 2.05%. Finally, the sharp line goes along temperature (X-axis) because of nickel oxide as residue. In Fe(III) complexes, the first step of degradation occurred in the range 71 – 183 ^oC, due to the loss of two coordinated water molecule with a practical weight 0.73% and 0.47%. The resultant complex on further degradation gave a break in the range 183 – 468 ^oC by the loss of phenyl group of Schiff base with practical weight 2.46% and 0.32%. Further, complex showed gradual decomposition up to 644 ^oC and onwards due to loss of remaining organic moiety. Finally, the metal oxide is remaining as a residue.

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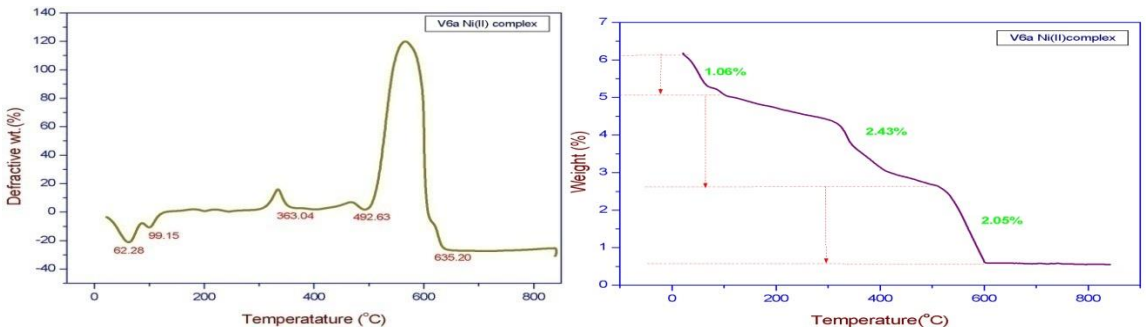
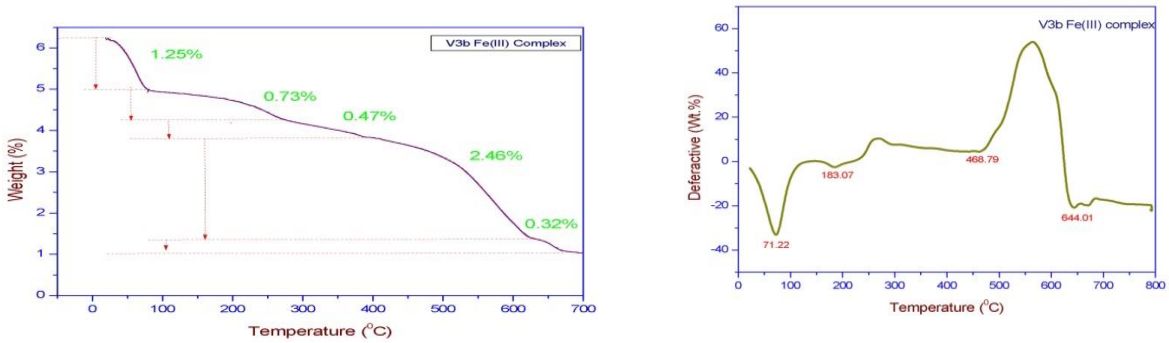


NiL2 complex.



$[FeL1(H_2O)_2]$ complex.

Figure 6. TGA – DTA of synthesized metal complexes.

3.8 Antibacterial activity

To contribute to the bioinorganic chemistry, In *vitro* evaluation of the antibacterial activity of the synthesized halo-Schiff base ligand and its metal complexes was carried out by screening them against given microorganisms. The respected microorganisms were standard strains of two gram-positive (*Bacillus cereus* and *Staphylococcus aureus*) and two-gram negative (*Pseudomonas aeruginosa* and *Escherichia coli*) pathogens. Synthesized compounds are active against strains of Gram-Positive as well as Gram-Negative bacteria. According to Overtones concept[42] and Tweedy's chelation theory[42], the antibacterial activity of metal complexes enhanced in comparison with the free ligands. From the reported data, it also clear that the Ni(II) and Fe(III) complexes are having more potent as Schiff base ligands.

Table 6. Antibacterial activity of Schiff bases ligand and metal complexes. (In mm)

Compound	***B. cereus***	***S. aureus***	***p. aeruginosa***	***E. coli***
(H_2L1)	20	24	11	08
(H_2L2)	21	22	10	09
[NiL1]	25	27	13	11
[NiL2]	27	24	12	10
[FeL1(H2O)2]	24	26	12	13
$[FeL2(H_2O)_2]$	27	29	14	07
Ampicillin	**26**	**27**	**14**	**11**

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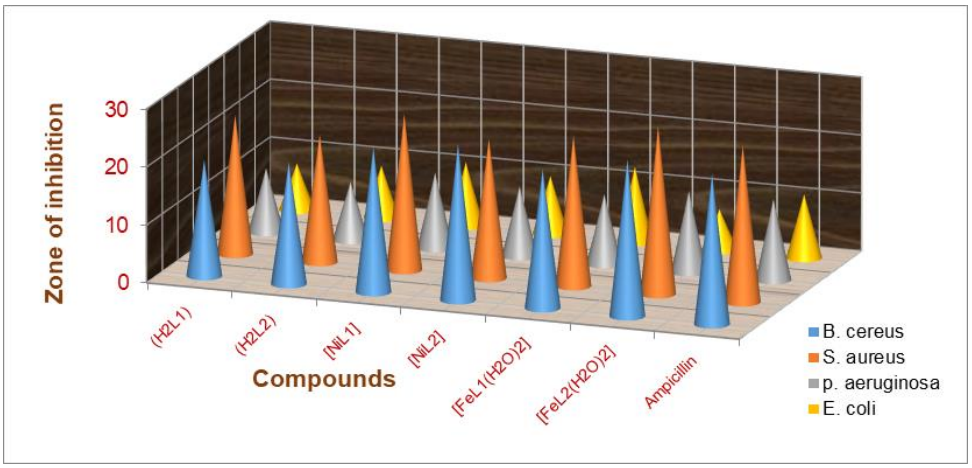

Figure 7. Antibacterial activity results of Schiff base ligand & metal complexes.

3.9 Antioxidant activity

The antioxidant activity of the Schiff base ligands and its metal complexes were evaluated by free radical scavenging activity by DPPH method comparison with standard butylated hydroxyanisole (BHA). The graphical representation is shown in figure 10. The results of the free radical scavenging activity of compounds at different concentrations are presented in table 7. Among these compounds, Ni(II) complexes showed good scavenging activity than Fe(III) complexes. The free ligands showed promising antioxidant activity as compared to all metal complexes, due to the presence of the phenolic –OH group.

Table 7. Antioxidant activity of Schiff bases ligand and metal complexes.

Compound	**12.5 *µ*g**	**25 *µ*g**	**50 *µ*g**	**100 *µ*g**
(H_2L1)	09.89±0.55	16.38±0.69	53.72±0.86	68.82±0.17
(H_2L2)	09.62±0.17	15.55±0.06	50.37±0.14	64.06±0.45
[NiL1]	08.42±0.05	13.71±0.17	48.11±0.08	59.13±0.35
[NiL2]	06.55±0.26	11.27±0.91	44.94±0.05	49.77±0.89
[FeL1(H2O)2]	06.85±0.12	09.28±0.50	28.73±0.29	37.46±0.57
[FeL2(H_2O)$_2$]	07.91±0.09	10.25±0.16	32.12±0.82	41.23±0.29
BHA	**11.31±0.62**	**18.44±0.67**	**58.18±0.67**	**72.12±0.88**

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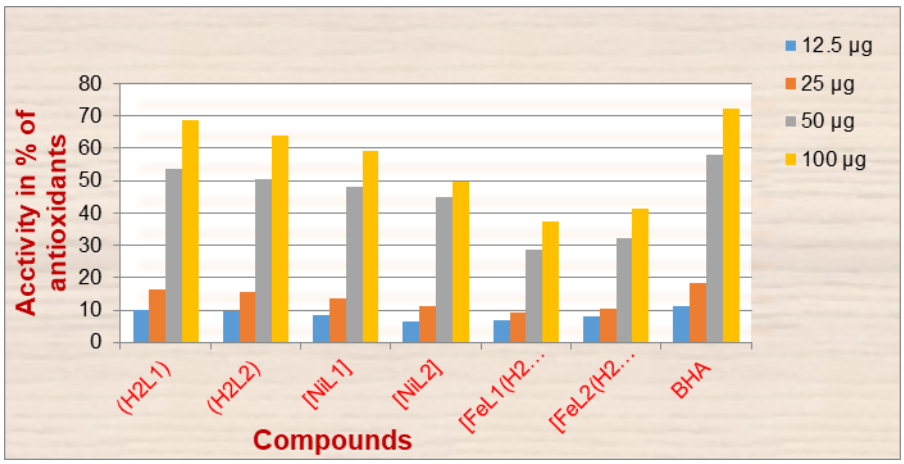

Figure 8. Antioxidant activity results of Schiff base ligand & metal complexes.

Conclusion

The present work has a series of Ni(II) and Fe(III) complexes were prepared with tetradentate N2O2 donor Schiff base ligands H_2L1 and H_2L2. They are characterized by various spectral techniques viz. UV Vis., FT-IR. ^{1}H NMR, ^{13}C NMR, and LCMS. Also, these metal complexes are studied by PXRD, TGA-DTA, and ESR analysis. From PXRD data, cognition of d-spacing values, FWHM, dislocation density, Crystallite size, and micro strain of synthesized metal complexes. The physico-chemical results demonstrate that Ni(II) complexes has a distorted square planar geometry and Fe(III) complexes has a octahedral geometry through involvement of naphthol oxygen and azomethine nitrogen. ESR studies support Fe(III) complexes which has a high spin *(d^5)* nature of the complexes. The antibacterial activity of all metal complexes showed potent antibacterial activity than ligands. The antioxidant activity of synthesized metal complexes is carried out with BHA as standard. The antioxidant activity of tetradentate Schiff base ligands is having more potency than metal complexes because of ligands having a free –OH group to reduce DPPH. Hence, from all these observations, it was concluded that the N2O2 tetradentate Schiff bases and its metal complexes gives versatile and valuable information of coordination compounds and also they may be used as good biological agents.

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Novel Co (II), Ni (II) Metal Complexes Derived from 1- Hydroxy-2-acetonaphthone Schiff Base: Synthesis, Characterization and Antimicrobial Evaluation

Bondar Dhananjay Vyankat*
Department of Chemistry, Shri Chhatrapati Shivaji College, Omerga, Dist. Osmanabad, Maharashtra, India
*E-mail- dvbondar21@gmail.com, Mobile no: +91 9420477636

Abstract

We present the synthesis, characterisation, and antibacterial activity of two new Co(II) and Ni(II) Schiff base metal complexes. The metal complexes were studied using UV-Vis, FT-IR, NMR, LCMS, ESR, and powder X-ray diffraction. UV-Vis. spectra revealed a more than 400 nm transition peak, confirming the occurrence of metal-ligand charge transfer. FT-IR reveals the production of an unsymmetrical Schiff base ligand and its complex including naphthol -OH and azomethine -C=N- groups. ^{1}H-NMR spectra confirm the production of the Schiff base ligand and its complexes. The XRD results confirm that the produced Co(II) and Ni(II) complexes have an orthorombic crystal structure. The ESR spectra of the Ni(II) complex indicated an octahedral geometrical arrangement surrounding the core metal ion. Schiff bases and their metal complexes exhibited antimicrobial efficacy against two-gram negative *E. coli, P. aeruginosa*, and two-gram positive *S. aureus, B. subtilis* bacterial strains. Schiff bases and metal complexes provide antifungal action against two fungus, *C. albicans and A. niger*. It was found that the derived complexes are more active than the comparable Schiff base.

Keywords: 1-Hydroxy-2-acetonaphthone, Phenylethyl amine, Schiff base, Metal complexes, Antimicrobial

1. Introduction

Nowadays, Schiff bases and the metal ion complexes that follow have drawn a lot of interest lately due to their many advantages. The usage of Schiff bases, which provide a range of effects and steric interactions with various geometries, has been extremely beneficial to the development of coordination chemistry [1]. Their varied catalytic, chemical, biological, and electrochemical properties make them a useful class of compounds that have been studied in great detail [2,3]. Through coordinative interactions with some or all of the donor atoms in the molecular structure, Schiff bases can coordinate many transition metal ions. They were systems with several donor sites that were either monodentate, bidentate, or polydentate [4,5]. Schiff base ligand-based transition metal complexes have just started to take centre stage in current research due to their popularity.

The utilization of naphthalene scaffold drugs presents significant benefits across a diverse array of pathophysiological disorders, encompassing antibacterial, antidepressant, anti-inflammatory, anti-cancer, and antiviral conditions [6]. Also, Naphthalene ring-based Schiff base compounds showed anti-COVID activity [7]. According to their different structural modifications, naphthalene moiety displays a wide spectrum of biological functions [8]. 1-Hydroxy-2-acetonaphthone (**HAN**) Schiff base metal complexes were described in the literature. The HAN Schiff base molecules were important in the development of food products [9]. The HAN has made substantially more attention to

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activities related to catalysis [10], dyes and pigments [11], antimicrobial [12], antiviral [13], anti-HIV [14], antioxidant [15], anticancer [16] and anti-inflammatory [17].
Cobalt has a lot of contribution in catalytic processes because of its redox active nature, particularly in olefin epoxidation and hydrocarbon oxidation [18]. Furthermore, complexes containing Ni(II) centres have exceptional magnetic characteristics due to the high spin of the metallic ion. Schiff base complexes with Co(II) and Ni(II) metals also observed in antioxidant activity [19]. Therefore, it appears, to our knowledge that there is no literature reporting the usage of these Schiff base compounds as the primary precursors to ensure their complexation with Co(II) and Ni(II) metals.

This report presents the synthesis and characterization of a Schiff base derived from HAN and phenylethylamine (**PEA**), along with its transition metal complexes, specifically Co(II) and Ni(II). Reported Schiff base and its metal complexes of Co(II), Ni(II) were illuminated by using the spectroscopic techniques like as UV-Vis., FT-IR, 1H-NMR, LCMS, Powder XRD and ESR study. Biological evaluation of Schiff base and its metal complexes of Co(II), Ni(II) were taken as an antibacterial activity towards *E. coli, P. aeruginosa* and *S. aureus, B. subtilis* microbes and antifungal activity for *C. albicans, A. niger fungus.*

2. Material and Methods

All analytical reagent grade chemicals, 1-Hydroxy-2-acetonaphthone, Phenylethyl amine, $Co(II)(OAc)_2{\cdot}4H_2O$ and $Ni(II)(OAc)_2{\cdot}4H_2O$ were purchased from Sigma Aldrich. From local vendors, we purchased HPLC grade methanol, absolute ethanol, other solvents and used without any purification. Thin layer chromatography (TLC) was used in laboratories to examine the purity of the products. TLC was done on 0.25-mm E Merck gel plates (60F-254) and the spots were seen under iodine vapours. Melting points were recorded using the Kofler bench a computerised device. The Perkin-Elmer 240 elemental analyzer was used to perform the elemental analysis. Shimadzu UV-1800 series spectrophotometer with 340 nm light source was used to record UV-visible spectra in methanol between 200-600 nm wavelength. FT-IR spectroscopy was examined the functional groups present in compounds, FT-IR spectra were taken with KBr disc on a Bruker Alpha II analyzer in the infrared spectrum between 650 and 4000 cm^{-1}. ^{1}H-NMR spectral data were collected using a Bruker AVANCE NEO 400 MHz spectrometer and $CDCl_3$ solvent with tetramethyl silane (TMS) serving as an internal reference standard. LCMS mass spectra of synthesised substances captured using a single quadrupole Agilent 1290 G7104A, model LCMSD G6125B MSD which having a scan range of 100 m/z to 1400 m/z. Powder XRD of ligand and metal complexes were recorded using a Desktop X-ray Diffractometer MiniFlex II with a range of 10 - 80^o target Cu and a wavelength of 1.540598 Å. ESR spectra of complex was captured using the JES-FA200 ESR spectrometer at a frequency of 9450.045 MHz and a power of 0.99500 mW.

Antibacterial activity

The Zone Inhibition Method was used to assess the antibacterial activity. In order to test the newly synthesised compounds antibacterial properties, bacteria including gram-negative *Escherichia coli, Pseudomonas aeruginosa* and gram-positive *Staphylococcus aureus, Bacillus subtilis* were utilised. After spreading and inoculating the Mueller Hinton Agar (MHA) plates with 100 µl of log cultures of each bacterium (adjusted to 0.5 McFarland Unit), the disc containing 10 µl of various concentrations (0 to 1000 mg/ml) were added. As a vehicle control, one disc in each plate was loaded with DMSO solvent alone and *Ciprofloxacin* (2 mg/ml, 20 µg) was used as the positive control. Clear zones surrounding the disc were measured and recorded after the test organism plates were incubated at 37°C for 24 hours.

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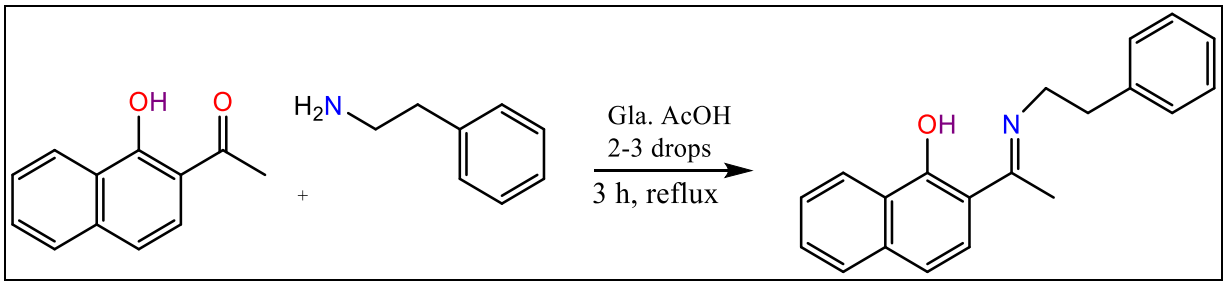
Antifungal activity

The Zone Inhibition Method was used to evaluate the anti-fungal activity. The freshly synthesised Schiff base and its metal complexes compounds were examined for their antifungal properties using the fungi *Candida albicans* and *Aspergillus niger*. The Zone Inhibition Method was used to evaluate the anti-fungal activity. 100 µl of log cultures from each of the two fungi strains were spread out and inoculated onto the Mueller Hinton Agar (MHA) and Potato Dextrose Agar (PDA) plates. Then putting the disc holding 10 µl of various concentrations (0 to 1000 g/ml) of *C. albicans, A. niger* respectively (adjusted to 0.5 McFarland Unit). Each plate had one disc that was solely loaded with DMSO solvent as the vehicle control. The *C. albicans* plates were incubated at 37°C for 24 hours and *A. Niger* plates were incubated for 24 to 74 hours at 32°C. We measured and noted the size of the disc in clear zone.

Synthesis of Schiff base ligand (HL)

According to the modified classical method as described in the literature, the Schiff base was prepared by dissolving of HAN (0.186 g, 1 mmol) in absolute ethanol (10 ml) then added 2-3 drops of glacial acetic acid. To this hot solution, ethanolic solution of PEA (0.120 g, 1 mmol) was added dropwise with constant stirring. Yellow coloured reaction mixture was refluxed around 3 hours and progress of rection was checked by TLC. For best result, reaction solution was kept overnight at ambient temperature. Lemon-yellow coloured fine needle shaped crystals (HL) were filtered off and recrystallised it using absolute ethanol.



Scheme 1 Synthesis of Schiff base ligand (HL)

2-(1-(phenethylimino)ethyl)naphthalen-1-ol (HL)

Molecular formula: [$C_{20}H_{19}NO$], Molecular weight: 289.38, Yield: 271.46 mg (87%), Colour: lemon-yellow, m. p. 122-124 ^{o}C. Elemental Analysis: C, 83.01; H, 6.62; N, 4.84; O, 5.53 FT-IR (KBr, cm^{-1}): 3424.01(ν -OH), 1703.14 (ν -C=N), 1591.53- 1452.91 (ν -C=C-), 1271.38 (ν -C-O), 1022.21(ν C-N-C). ^{1}H NMR (400 $CDCl_3$), δ (ppm): 2.255 (s, -CH_3, 3H), 3.107 (t, -CH_2-, 2H), 3.820 (t, N-CH_2, 2H), 6.774- 8.539 (m, Ar-H, 10H), 16.414 (s, Ar-OH, 1H). *ESIMS* (m/z): 290.2

Synthesis of metal complexes [$M(L)_2$]

According to the published literature general procedure for synthesis of Co(II) and Ni(II) complexes were observed. Metal salts 1 mmol, 0.249 g for Co(II)$(OAc)_2 \cdot 4H_2O$ and 0.248 g for Ni(II)$(OAc)_2 \cdot 4H_2O$ were dissolved in methanol solvent and it was added into a Schiff base (HL) hot methanolic solution, immediately colour of the solution changes which indicates ligand metal

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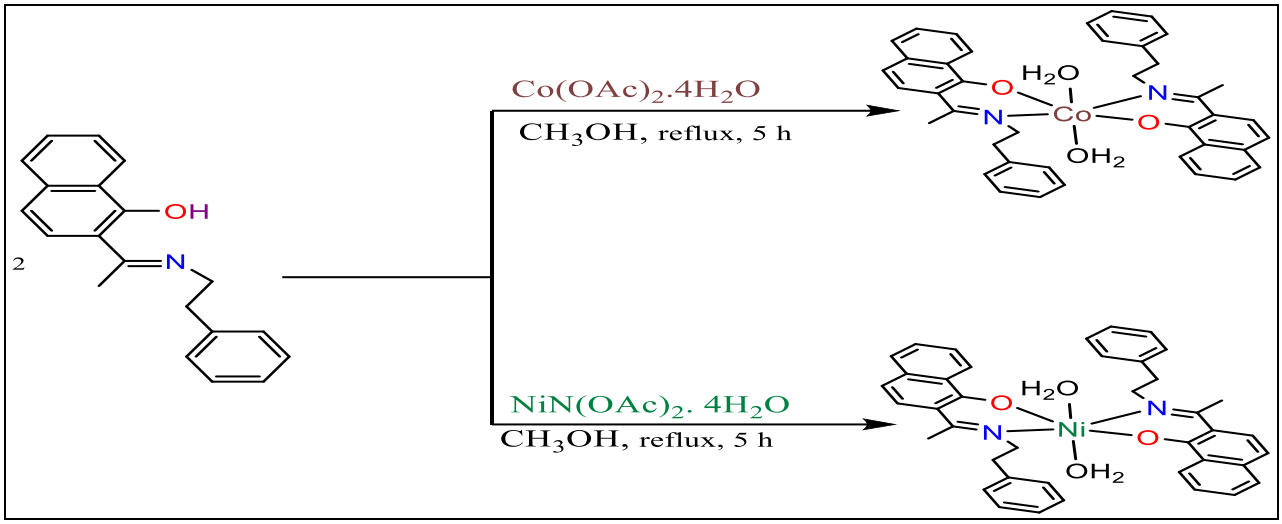
complexation. Then, the reaction mixture was refluxed for 5 hours and after completion the reaction solution was cooled at room temperature. The resultant solid was filtered off and then extensively cleaned with dry diethyl ether and a little amount of methanol.



Scheme 2 Synthesized Metal complexes $M(L)_2$

$Co^{II}(L)_2$ complex $[Co(L)_2(H_2O)_2]$

Molecular formula: $C_{40}H_{40}CoN_2O_4$, Molecular weight: 668.62, Yield: 541 mg (65%), Colour: Brown red, m. p. 251- 253 °C. Elemental Analysis: C, 71.53; H, 6.01; Co, 8.47; N, 4.26; O, 9.51

FT-IR (KBr, cm^{-1}): 1616.92 (ν C=N), 1577.72- 1452.02 (ν C=C), 1250.38 (ν C-O), 1024.19 (ν C-N-C). ^1H NMR (400, $CDCl_3$), δ (ppm): 2.709 (s, $-CH_3$, 3H), 3.499 (t, $-CH_2$, 2H), 3.527 (t, N-CH_2, 2H), 7.260- 8.475 (m, Ar-H, 10H). *ESIMS* (m/z): 671.70 (100.0%).

$Ni^{II}(L)_2$ complex $[Ni(L)_2(H_2O)_2]$

Molecular formula: $C_{40}H_{40}NiN_2O_4$, Molecular weight: 667.24, Yield: 490 mg (59%), Colour: Olive, m. p. 176- 178 °C. Elemental Analysis: C, 71.84; H, 6.02; Ni, 8.38; N, 4.28; O, 9.62

FT-IR (KBr, cm^{-1}): 1591.50 (ν C=N), 1526.55- 1452.88 (ν C=C), 1270.98 (ν C-O), 1022.10 (ν C-N-C). ^1H NMR (400, $CDCl_3$), δ (ppm): 2.288 (s, $-CH_3$, 3H), 3.106 (t, $-CH_2$, 2H), 3.827 (t, N-CH_2, 2H), 6.786- 8.536 (m, Ar-H, 11H). *ESIMS* (m/z): 670.23 (100.0%).

Table 1 Analytical and physical data of ligand and its metal complexes

Sr. no.	Compound	Colour	Yield %	m.pt .(°C)	Elemental Analysis found (Cal.) %				
					C	H	N	O	M
1	HL, $C_{20}H_{19}NO$	lemon-yellow	82	132-134	83.01 (82.97)	6.62 (6.59)	4.84 (4.81)	5.53 (5.49)	-
2	$Co(L)_2{\cdot}(H_2O)_2$	Brown	67	291-293	71.53 (71.81)	6.01 (5.97)	4.26 (4.13)	9.51 (9.49)	8.47 (8.27)

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3	$Ni(L)_2 \cdot (H_2O)_2$	Green	63	216-218	71.84 (71.91)	6.02 (5.95)	4.28(4.12	9.62 (9.56)	8.38 (8.14)

Results and discussion

The synthesized Schiff base and metal complexes come in a variety of hues and are stable at ambient temperature in both air and moisture. They dissolve in chloroform, dichloromethane, dimethyl sulfoxide, dimethylformamide, tetrahydrofuran, ethyl acetate, acetone and insoluble in petroleum ether, n-hexane. They were structurally confirmed by UV-Vis., FT-IR spectra,^{1}H NMR, Powder XRD, ESR and LCMS.

UV-Vis. Analysis

The Schiff base ligand (HL) and its metal complexes UV-Visible absorption spectra were recorded in a methanol solvent. The Schiff base has five main peaks that was located at ranges of 225.50, 271.50, 322.50, and 409.00 nm. The aromatic ligand ring transition at 225–300 nm causes the bands. The bands between 300 and 350 nm was triggered by the ligand chromophore (-C=N-) $\pi \rightarrow \pi^*$ transition. The intramolecular charge interactions of $n \rightarrow \pi^*$ transition of non-bonding electrons present on the Schiff base compound were responsible for the extended wavelength bands exceeding 400 nm [20]. Also, in the Co (II), Ni(II) metal complexes wavelength seen more than 400 nm which were pushing electronic absorption band because of metal ligand charge transfer (MLCT) transitions.

FT-IR analysis

We are able to understand how the coordination between the metal ion and ligand was achieved by using FT-IR analysis of the recently produced Schiff base and its complexes as shown in Fig. 1, 2. The ligand displays a prominent band with a strong center at 3424.01 cm^{-1} indicating the presence of a phenolic (Ph-OH) group with extensive intra-intermolecular hydrogen bonding. Schiff base ligand imine peak (-C=N-) was shown at range 1703.14 cm^{-1}. Aromatic (-C=C-) peaks range was observed from 1591.53- 1452.91 cm^{-1} and aromatic (Ar-H) small intensity peaks at range 3029.89-2866.55 cm^{-1}. When compared to metal complexes IR spectra broad peak Phenolic -OH was disappeared which concluded deprotonation of ligands phenolic -OH group. When imine (-C=N-) group participating in bonding with metal ions, it was shifted towards lower frequency at 1616.92 cm^{-1}, 1591.50 cm^{-1} for Co(II), Ni(II) metal complexes respectively.

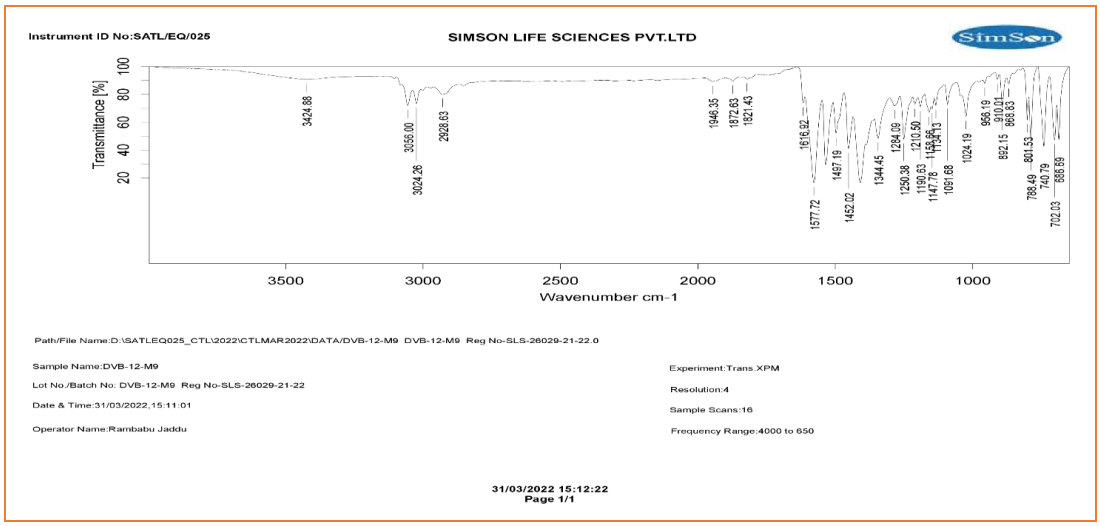

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Fig. 1. IR spectra of $[Co(L)_2(H_2O)_2]$ complex

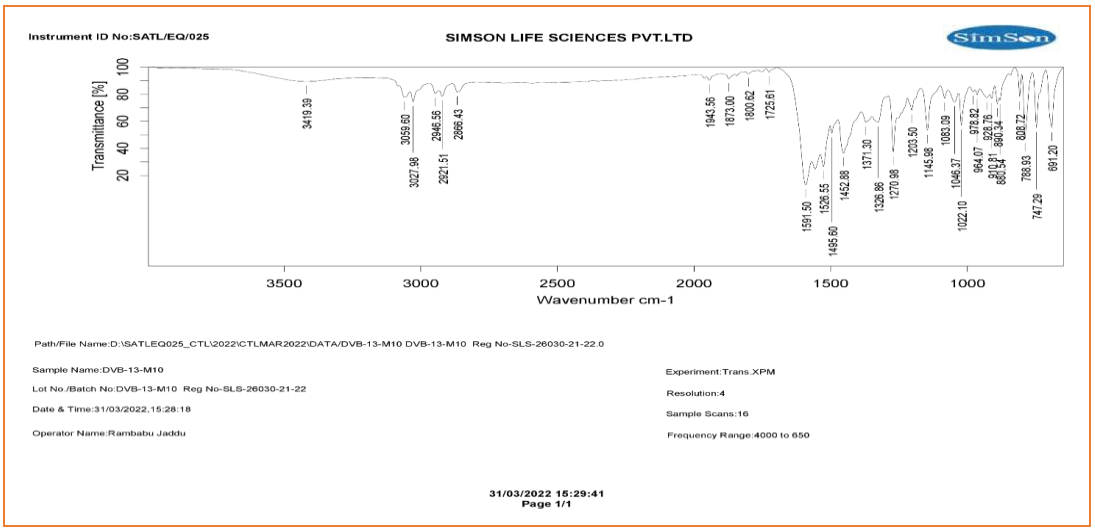

Fig. 2. IR spectra of $[Ni(L)_2(H_2O)_2]$ complex

Table 2 FT-IR spectral data of Schiff base and its complexes

Compound	ν(-OH)	ν(H_2O)	ν(C=C–H)	ν(C=N–)	ν(C–O)	ν(C-N-C)
HL	3424.01	-	3059.89	1591.53	1271.38	1022.21
$Co(L)_2(H_2O)_2$	-	3424.88	3056.00	1616.92	1250.38	1024.19
$Ni(L)_2(H_2O)_2$	-	3419.39	3059.60	1591.50	1270.98	1022.10

^{1}H NMR analysis

In ^{1}H NMR spectra of the ligand HL, the proton of phenolic -OH was discernible as a singlet at 16.414 ppm. For Schiff base ligand and its metal complexes, aromatic proton signals resonate as multiplate in the 6.627-8.869 ppm range. Two triplet signals of the ethylene chain =N-CH_2- CH_2-Ar were seen at 3.820, 3.107 ppm in the ligand while these triplet signals were seen downfield in the metal chelates. The peak at 2.255 was caused due to methyl protons of the ligand with the formula -N=C-CH_3 and this peak was marginally impacted by metal chelates [21]. In contrast to the ^{1}H NMR spectra of the ligand and its metal complexes, the protons signals have been shifted towards the downfield, which is a proof that metal ion has complexed with the ligand.

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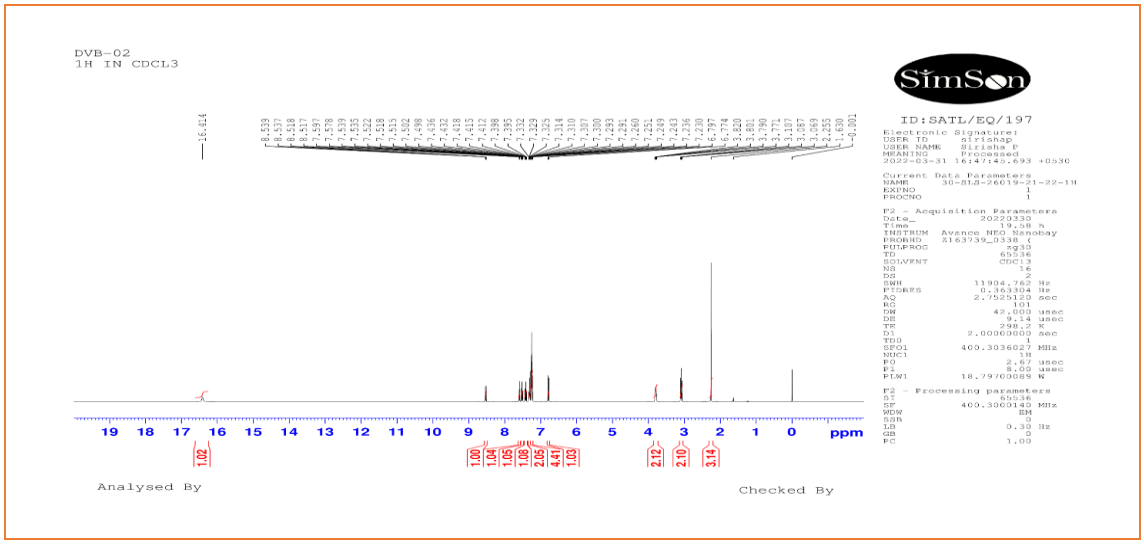

Fig. 3. ^{1}H NMR spectra of Schiff base ligand (HL)

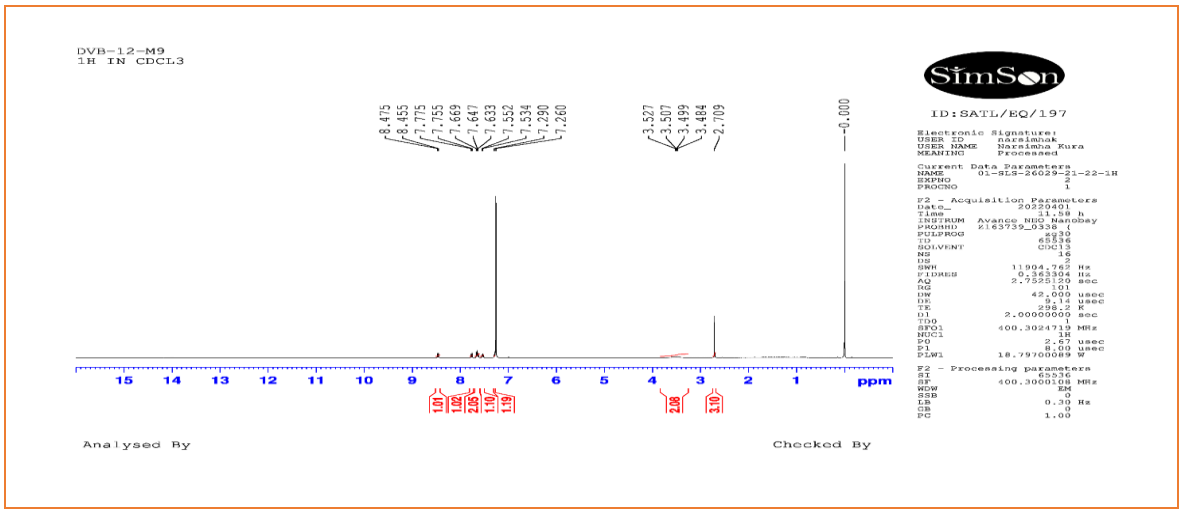

Fig. 4. ^{1}H NMR spectra of $[Co(L)_2(H_2O)_2]$ complex

LC-MS

The ESI- MS analysis verified the Schiff base ligand and related metal complexes molecular weights as shown in Fig. 5- 7. The Schiff base ligand HL was showed a molecular ion peak at m/z 290.2, which is equivalent to its molecular weight. Similar molecular ion peak was observed in related metal complexes which confirms the association of ligand with metal ions and fragmented when taking mass spectra. Metal complexes $[Co(L)_2(H_2O)_2]$, $[Ni(L)_2(H_2O)_2]$ were associated with the molecular ion peaks at m/z 748.23, 747.24 respectively.

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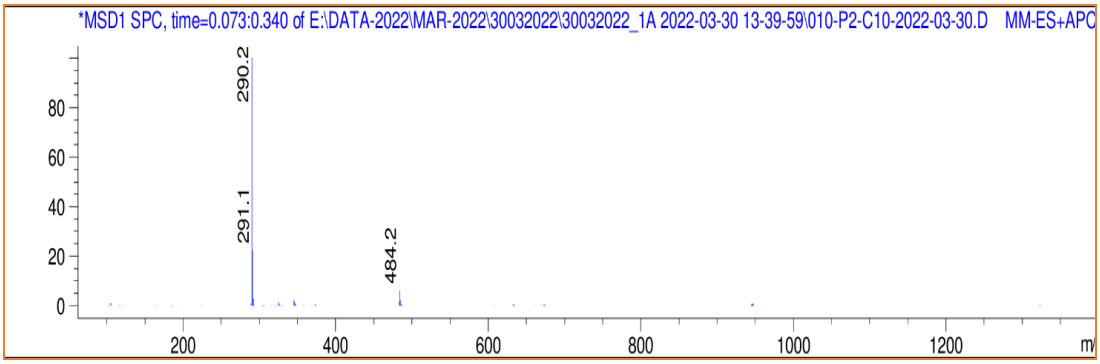

Fig. 5. Mass spectra Schiff base ligand (HL)

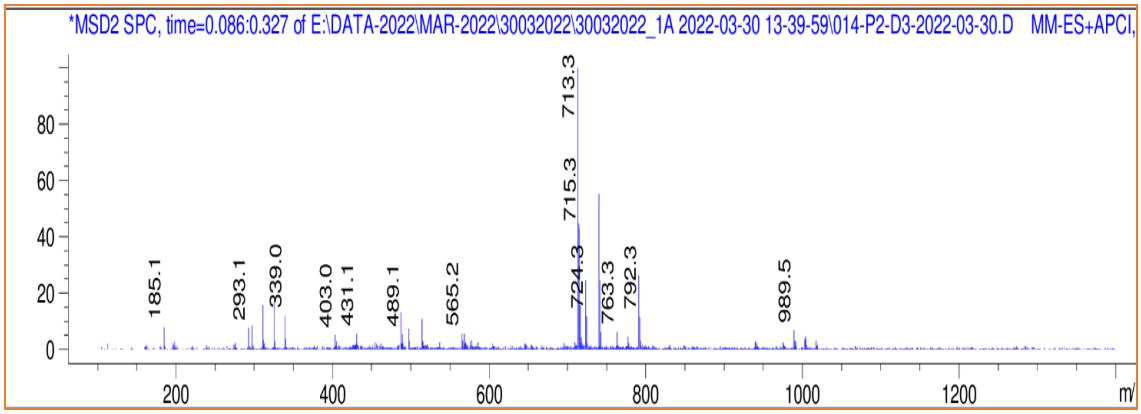

Fig. 6. Mass spectra of $[Co(L)_2(H_2O)_2]$ complex

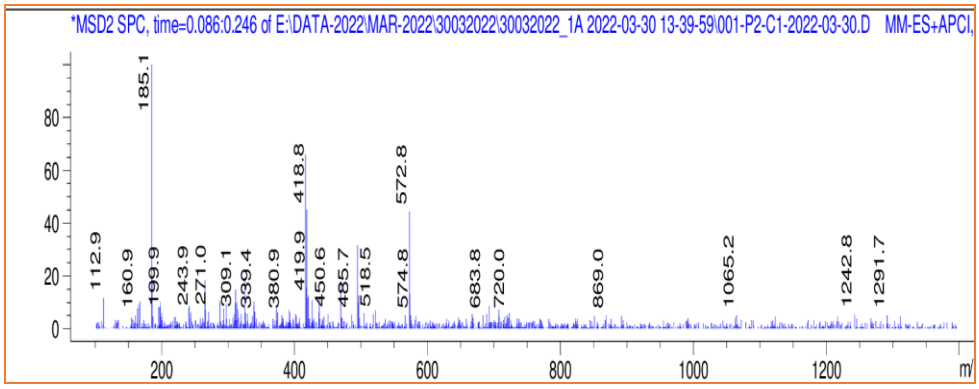

Fig. 7. Mass spectra of $[Ni(L)_2(H_2O)_2]$ complex

Powder XRD

The powder X-ray diffractometer was used to carry out the analysis, which had the following settings; scanning mode: 2θ/θ, scanning type: continuous and scan speed: 5.000 deg./min. Fine X-ray peaks as in Fig. 8, 9 were assigned to the synthesised ligand and its complexes which helped with comparison and the creation of metal complexes with the Schiff base ligand. From the XRD graphs, intensity of ligand peaks were decreased in the metal complexes and peaks broadness were increased in metal chelates; this indicates the existence of ligand metal chelation [22]. We discovered the ligand and complexes from the XRD analysis, its crystal system, space group, and unit cell volume parameters which are shown in Table 3.

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Table 3 Powder-XRD data of Schiff base and its metal complexes

Compound	HL	$[Co(L)_2(H_2O)_2]$	$[Ni(L)_2(H_2O)_2]$
Empirical formula	$C_{20}H_{19}NO$	$C_{40}H_{40}CoN_2O_4$	$C_{40}H_{40}NiN_2O_4$
Formula weight	289.38	671.70	671.46
Temperature, K	298	298	298
Crystal system	Tetragonal	Orthorombic	Orthorombic
Lattice type	P1	P1	P1
a/A°	5.250244	16.11380	9.430661
b/A°	5.250244	13.67799	7.383021
c/A°	25.42294	5.843458	7.258832
α/°	90.00000	90.00000	90.000000
β/°	90.00000	90.00000	90.00000
γ/°	90.00000	90.00000	90.000000
Unit cell volume, $A^{\circ 3}$	448.4194	936.4671	867.74183

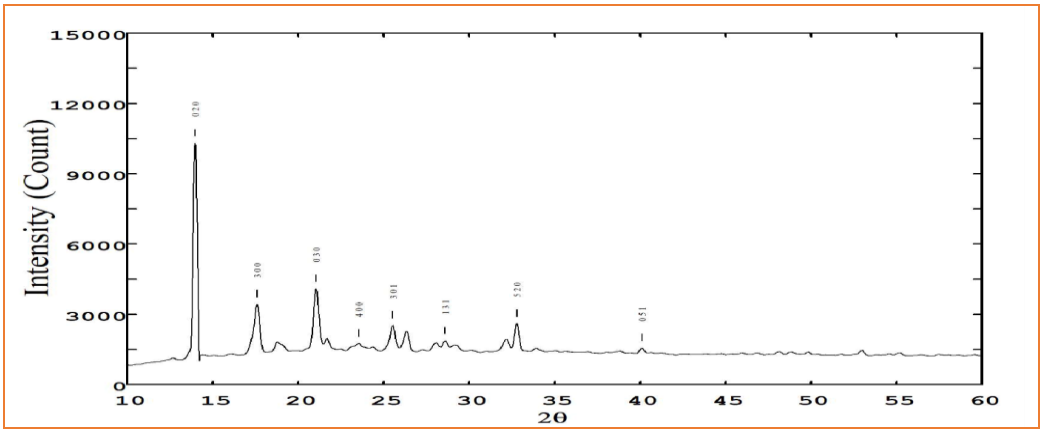

Fig. 8. XRD spectra of $[Co(L)_2(H_2O)_2]$ complex

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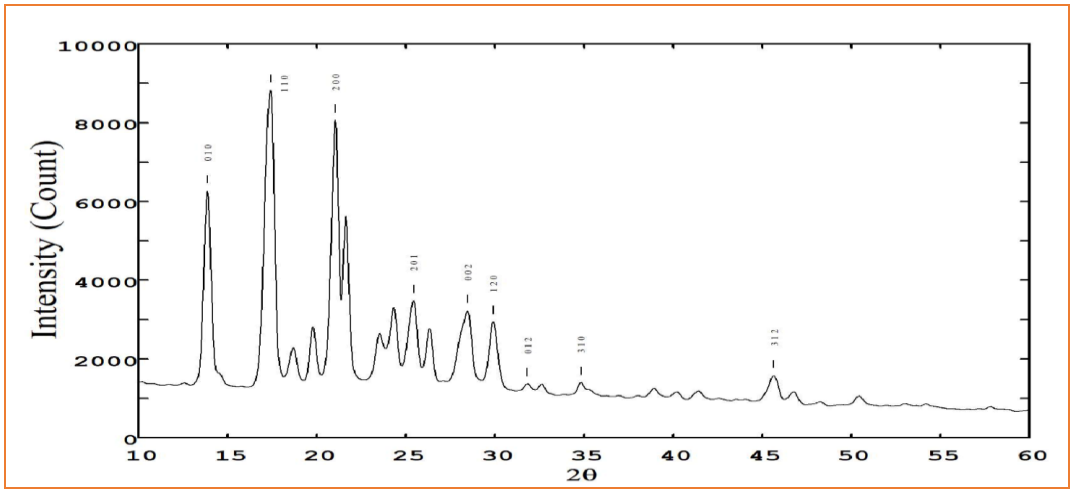

Fig. 9. XRD spectra of $[Ni(L)_2(H_2O)_2]$ complex

ESR spectral analysis

The solid Co(II) complex X-band ESR spectra was displayed in Fig. 10, the broad signal and lack of hyperfine structure points out excellent coupling between the spin system and lattice vibrations as well as low spin relaxation with g|| = 2.0538 and g⊥ value 2.00864, average g value calculated by equation $g_{av} = \frac{g||+2g\perp}{3}$ is 2.02369. Here, g|| is less than 2.3, suggesting that the Co-L bond is covalent and octahedral geometry [23].

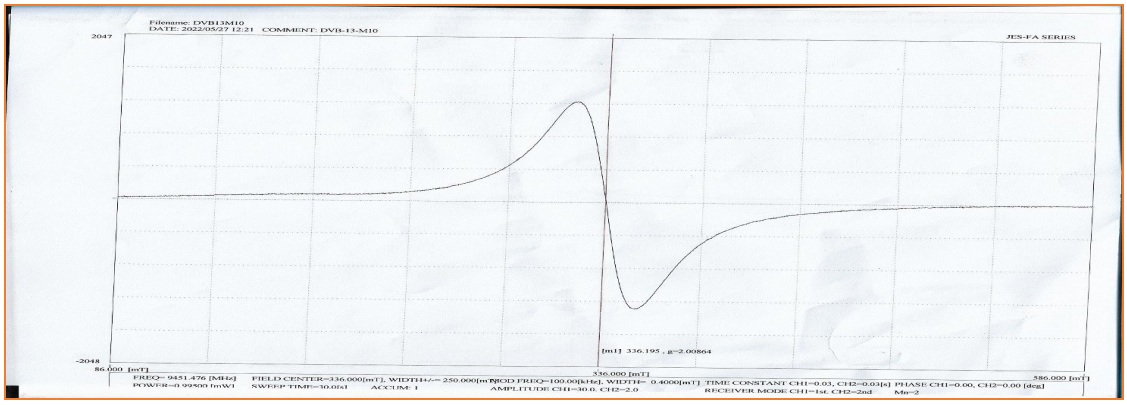

Fig. 10. ESR spectra of $[Co(L)_2(H_2O)_2]$ complex

Antimicrobial activity

In vitro antibacterial activity of Schiff base ligand and complexes were explored as shown in Table 4. To enhance bioinorganic chemistry, *in vitro* tests of the synthesised Schiff base ligand and their metal complexes antibacterial properties were conducted by screening them against specified pathogens. These specific microorganisms included in conventional strains of two gram-negative *Escherichia coli*, *Pseudomonas aeruginosa* as well as gram-positive bacteria *Staphylococcus aureus*, *Bacillus subtilis*. Metal complexes have more antibacterial activity than free ligand, according to Tweedy's chelation theory and Overtone's idea [24]. *In vitro* antifungal activity of Schiff base ligand and complexes were investigated as shown in Table 4. Mueller Hinton Agar and Potato dextrose agar was used to cultivate the fungi *Candida albicans* and *Aspergillus niger* respectively. Both antifungal

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tests for Schiff base ligand and metal complexes display more activity than *Ciprofloxacin* as the reference medication. Additionally, when HL ligand was chelated with metals, its antifungal bioactivity increases. Thus, it can be said that metal complexes show greater inhibition of the taken micro organisms development.

Table 4 *In vitro* Antibacterial and Antifungal activity data of Schiff base and its metal complexes (in mm)

Compound	Concentration µg/ml	Antibacterial activity				Antifungal activity	
		E. coli	P. aeruginosa	S. aureus	B. subtilis	C. albicans	A. niger
HL	1000	9	10	12	8	6	8
	500	9	8	9	8	6	6
	250	7	7	7	7	5	6
	125	6	7	6	-	-	5
	50	-	6	-	-	-	-
$[Co(L)_2(H_2O)]$	1000	15	13	14	15	11	13
	500	11	12	8	13	9	10
	250	8	7	6	8	6	6
	125	5	4	5	6	4	5
	50	-	-	-	-	-	-
$[Ni(L)_2(H_2O)]$	1000	15	15	13	14	15	15
	500	13	12	11	13	13	12
	250	8	9	9	12	7	8
	125	6	7	7	8	6	-
	50	-	-	-	-	-	-
*Ciprofloxacin**	20	39	31	33	28	5	5

*- reference drug

Conclusion

In light of the current study, a novel Schiff base 2-(1-(phenethylimino)ethyl)naphthalen-1-ol (HL) was synthesized and characterized by the condensation of 1-Hydroxy-2-acetonaphthone and Phenylethyl amine. UV-Vis, FT-IR, and ^{1}H NMR spectroscopy were used to suggest the formation of

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the ligand and its complexes. The bidentate ligand HL contains N and O donor atoms and binds to metal ions. It was also demonstrated using LCMS mass spectra, powder XRD, and ESR spectrum analysis. Metal complexes were observed to have an octahedral geometry. When the ligand was absent, Schiff bases had poor bioactivity; however, when coupled with metal atoms, they have outstanding antibacterial bioactivity. As a result, naphthalene-based chemicals and their complexes have high biological activity. The existing sequence of chemicals should be enhanced and evolved into primary molecules. As a result, the current study is valuable in developing a new class of antibacterial and antifungal medications.

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Isolation, Characterization and identification of Phosphate SolubilisingBacteria, Bacillus megaterium Ra-Fi7 from Agricultural Soil of LaturRegion, Maharashtra

F.S. Biradar,[1,] V.S. Shembekar[2]
[1] Assistant Professor, Department of Biotechnology DSC, Latur.
[2] Retd. Professor, Department of Zoology R.S. College Latur.

Abstract

The present study aimed to isolate, characterize, and identify a potential Phosphatesolubilising bacteria Bacillus megaterium, a prominent Gram-positive bacteriumwithsignificant industrial, agricultural, and environmental applications. Soil samples werecollected from various agricultural fields with the objective of isolating bacterial strainscapable of contributing to biofertilization and bioremediation processes. The isolationprocessinvolved the use of selective media that supported the growth of B. megaterium, ensuringthesuccessful separation of this microorganism from the native microbial population. Initial characterization included morphological observation, where colonies exhibited large, creamy-white, circular appearances typical of B. megaterium. Microscopic examination confirmedthe presence of large, rod-shaped cells, and Gram-staining verified their Gram-positive nature. Further biochemical tests, including catalase production, starch hydrolysis, andnitratereduction, aligned with the expected profile of B. megaterium. The bacterium's abilitytoproduce extracellular enzymes like protease and amylase was evaluated, indicatingitspotential in industrial enzyme production. For molecular identification, 16S rRNAgenesequencing was employed, confirming the isolate as Bacillus megaterium. Phylogeneticanalysis also supported the identification by placing the isolate within the Bacillus genus. Theversatility of B. megaterium in producing bioactive compounds, along with its abilitytosurvive in extreme conditions, highlights its potential for applications in agricultureasabiofertilizer and in environmental sectors as a bioremediating agent. This study not onlyadvances the understanding of Bacillus megaterium in biotechnological and ecological settings but also opens new avenues for further exploration of its beneficial rolesinsustainable agricultural practices and environmental management. Keywords: Bacillus megaterium, isolation, characterization, identification, 16SrRNAsequencing, biofertilizer, bioremediation, enzyme production, soil bacterium, Agricultural Microbiology.

1. Introduction

Microorganisms play a crucial role in various ecosystems, particularly in agricultureandindustry, due to their diverse metabolic capabilities and their ability to adapt to a wide rangeof environmental conditions (Singh et al., 2020). Among them, Bacillus megaterium, aGram-positive, rod-shaped bacterium, has garnered significant attention for its wide rangeofindustrial applications, including enzyme production, biofertilization, and bioremediation (Kumar et al., 2021). Isolated from soil, B. megaterium is known for its large cell size andtheproduction of various extracellular enzymes, making it a valuable microorganismin industrial processes (Turan et al., 2019). In agricultural practices, B. megaterium has been recognized for its ability to promoteplant growth by solubilizing phosphorus, producing phytohormones, and enhancingnutrient availability in the soil (Choudhary et al., 2022). This bacterium can also fix nitrogen, contributing to soil fertility and improving crop yield without the need for synthetic fertilizers, making it an eco-friendly alternative (Goswami and Kalita, 2020). Moreover, B. megateriumshows potential for bioremediation, particularly in the degradation of toxic compounds suchas heavy metals and pesticides, thus

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contributing to environmental sustainability (Rana et al., 2021). The identification and characterization of B. megaterium fromvarious soil samplescan help expand its applications in industrial and agricultural sectors. Traditional methods, such as morphological and biochemical tests, are commonly used for bacterial identification. However, molecular techniques, such as 16S rRNA gene sequencing, provide more accurateand reliable results for distinguishing bacterial species (Jain and Sharma, 2020). This studyfocuses on the isolation, characterization, and identification of Bacillus megateriumfromagricultural soil, emphasizing its potential applications in biofertilizer productionandbioremediation.

2. Materials And Methods

1. Sample Collection

Soil samples were collected from agricultural fields located in [Latur region,Maharashtra]. Using sterile tools, approximately 10-15 grams of soil were collected at a depth of 5-10cm. The samples were placed in sterile containers and transported to the laboratory for furtheranalysis. Soil samples were stored at 4^0C until processing.

2. Isolation of Bacterial Strains

To isolate Bacillus megaterium, serial dilution and spread plate methods were employed. Tengrams of soil were suspended in 90 mL of sterile distilled water and vortexed for 10 minutes. Serial dilutions (up to 10^{-6}) were prepared, and 100 µL of each dilution was spreadontoNutrient Agar (NA) plates. Plates were incubated at 30^0C for 24-48 hours. Coloniesexhibiting large, circular, cream-colored morphology were selected for further studies.

3. Morphological Characterization

Morphological features of the selected bacterial colonies were observed using standardtechniques. Gram staining was performed to determine the Gram reaction, and cell shapeandsize were examined under a light microscope (100x magnification). Colony characteristics, such as size, shape, color, and margin, were recorded.

4. Biochemical Characterization

The bacterial isolates were subjected to a series of biochemical tests to confirmthe identityofBacillus megaterium. These tests included:

- Catalase Test: A drop of 3% hydrogen peroxide was added to a bacterial smear toobserve the release of oxygen bubbles, indicating a positive reaction.
- Starch Hydrolysis Test: Bacteria were inoculated on starch agar plates and incubatedfor 24 hours. After incubation, the plates were flooded with iodine solution, andclearzones around the colonies indicated positive starch hydrolysis.
- Nitrate Reduction Test: Nitrate broth was inoculated with the bacterial cultureandincubated at 30^0C for 24 hours. The addition of nitrate reagents was followedbyobservation for a color change, indicating the reduction of nitrate to nitrite.
- Other tests: Additional tests, including the citrate utilization test, indole production, and gelatin hydrolysis, were conducted as per standard protocols (CappuccinoandSherman, 2014).

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5. Molecular Identification using 16S rRNASequencing

Molecular identification of the isolated bacterium was performed using 16S rRNAgenesequencing. Genomic DNA was extracted using a bacterial DNA extraction kit (e.g., Qiagen) following the manufacturer's instructions. The 16S rRNA gene was amplified using universal primers (27F and 1492R). PCR conditions were optimized with an initial denaturationat 94 0C for 5 minutes, followed by 35 cycles of denaturation at 94 0C for 30 seconds, annealingat 55 0C for 30 seconds, and extension at 72 0C for 1 minute. The final extension was carriedout at 72 0C for 5 minutes. The amplified products were visualized using agarosegel electrophoresis (1.5%), and successful amplicons were sent for sequencing. The sequencesobtained were compared with existing sequences in the NCBI database using BLASTforspecies identification. The resulting 16Sr RNA gene sequences were submitted to DDBJ.

6. Phylogenetic Analysis

The 16S rRNA sequence of the isolated strain was aligned with reference sequences fromtheNCBI database using the ClustalW algorithm. A phylogenetic tree was constructed usingtheneighbor-joining method in MEGA X software to determine the evolutionary relationshipofthe isolate with closely related Bacillus species.

7. Phosphate Solubilization

a) Media Preparation:

Pikovskaya's agar medium containing tricalcium phosphate was used to evaluatephosphate solubilization potential.

b) Culture Inoculation:

A single colony of Bacillus megaterium was picked with a sterile toothpickandplaced on the Pikovskaya's agar plate.

c) Incubation:

The plates were incubated at 30 ± 1°C for seven days.

d) Phosphate Solubilization Index (SI):

The SI was calculated using the formula:

SI = (Colony diameter + Halo zone diameter) / Colony diameter

The study reported a solubilization index (SI) of 3.0 ± 0.1 for the isolate.

8. Enzyme Production Assay

To assess the industrial potential of the isolated strain, enzyme production was evaluated. Protease and amylase production assays were performed using skim milk agar and starchagarplates, respectively. The plates were incubated at 30^0C for 24-48 hours. Zones of clearancearound the colonies indicated the production of protease and amylase. 3

9. Statistical Analysis

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All experiments were performed in triplicate, and the results were expressed as mean±standard deviation (SD). Data were analyzed using Microsoft Excel, and statistical significance was evaluated using a one-way ANOVA test where applicable, with a p-value<0.05 considered significant.

Results

Isolation and Morphological Characterization

The bacterial colonies isolated from the soil samples on Nutrient Agar (NA) plates weredistinct, exhibiting large, circular, and cream-colored morphology, characteristic of Bacillusmegaterium. Under a microscope (100x magnification), Gram staining revealed largerod-shaped, Gram-positive cells. The colony and cell characteristics are summarized in Table1.

Table 1: Morphological Characteristics of Isolated *Bacillus megaterium*

Characteristic	Observation
Colony shape	Circular
Colony color	Cream
Colony size	Large (~3-4 mm diameter)
Gram reaction	Positive
Cell shape	Rod-shaped
Cell size	Large (2-3 µm in length)

Table 1: Morphological Characteristics of Isolated Bacillus megaterium

Characteristic	Observation
Colony shape	Circular
Colony color	Cream
Colony size	Large (~3-4 mm diameter)
Gram reaction	Positive
Cell shape	Rod-shaped
Cell size	Large (2-3 µm in length)

2. Biochemical Characterization

The isolate was subjected to standard biochemical tests. It tested positive for catalase, starchhydrolysis, and nitrate reduction, while it showed negative results for indole productionandcitrate utilization. These results align with the known biochemical profile of Bacillus megaterium. The findings are presented in Table 2.

Table 2: Biochemical Test Results for Bacillus megaterium

Biochemical Test Result	Catalase Positive

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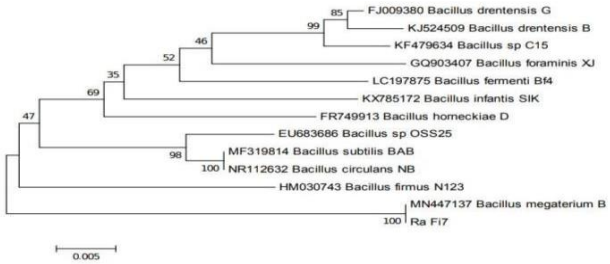
Starch hydrolysis	Positive
Nitrate reduction	Positive
Citrate utilization	Negative
Indole production	Negative
Gelatin hydrolysis	Positive

3. Molecular Identification

The molecular identification of the isolate was confirmed by 16S rRNAgene sequencing. The amplified gene fragment was approximately 1,500 bp in length. A BLASTsearchof theNCBI database revealed a 99% sequence similarity with known Bacillus megateriumstrains, confirming the identity of the isolate.

4. Phylogenetic Analysis

Phylogenetic analysis, based on the 16S rRNA sequence, placed the isolated strain in close relation to other Bacillus megaterium strains. The neighbor-joining tree showed clustering with previously identified Bacillus megaterium strains, confirming its genetic similarity (Figure 1 –phylogenetic tree).



>*Bacillus megaterium Ra-Fi7*
TGAGTAACACGTGGGCAACCTGCCTGTAAGACTGGGATAACTTCGGGAAACCGAAGCTA
ATACCGGATAGGATCTTCTCCTTCATGGGAGATGATTGAAAGATGGTTTCGGCTATCACTT
ACAGATGGGCCCGCGGTGCATTAGCTAGTTGGTGAGGTAACGGCTCACCAAGGCAACGA
TGCATAGCCGACCTGAGAGGGTGATCGGCCACACTGGGACTGAGACACGGCCCAGACT
CCTACGGGAGGCAGCAGTAGGGAATCTTCCGCAATGGACGAAAGTCTGACGGAGCAAC
GCCGCGTGAGTGATGAAGGCTTTCGGGTCGTAAAACTCTGTTGTTAGGGAAGAACAAGT
ACGAGAGTAACTGCTCGTACCTTGACGGTACCTAACCAGAAAGCCACGGCTAACTACGTG
CCAGCAGCCGCGGTAATACGTAGGTGGCAAGCGTTATCCGGAATTATTGGGCGTAAAGCG
CGCGCAGGCGGTTTCTTAAGTCTGATGTGAAAGCCCACGGCTCAACCGTGGAGGGTCAT
TGGAAACTGGGGAACTTGAGTGCAGAAGAGAAAAGCGGAATTCCACGTGTAGCGGTGA
AATGCGTAGAGATGTGGAGGAACACCAGTGGCGAAGGCGGCTTTTTGGTCTGTAACTGA
CGCTGAGGCGCGAAAGCGTG

5. Determination of Phosphate Solubilizing Index (SI)

Phosphate solubilizing index of this isolate showing clear zone formation around the colony were determined using the Pikovskayas Agar Media (PKV) agar media containing Tricalcium phosphate (Gupta etal.1994). A single colony of pure active culture was picked up with the help of sterilized toothpick and placed on the plate and incubated at 30± 1 ˚C for 7 days. Solubilization Index (SI) was calculated by using formula (Edi –premono et al., 1996).

SI = colony diameter + halo zone diameter / Colony diameter.

SI of Bacillus megaterium = 3.0± 0.1

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6. Enzyme Production Assay

To assess the industrial potential of the isolated Bacillus megaterium, enzyme production assays were performed for protease and amylase. Significant zones of clearance were observed around the colonies on skim milk agar and starch agar plates, indicating protease and amylase activity, respectively. The enzyme activity was measured based on the diameter of the clearance zones, as shown in Table 3.

Table 3: Enzyme Production Results for *Bacillus megaterium*

Enzyme	Zone of Clearance (mm)
Protease	18.5 ± 0.8 mm
Amylase	23.2 ± 1.1 mm

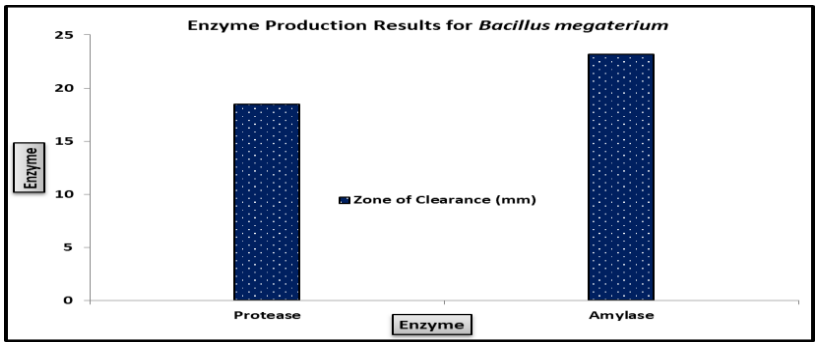

Figure 2: Enzyme Production Results for *Bacillus megaterium*

6. Statistical Analysis

The enzyme production data were analyzed statistically, and the results are expressed as mean ± standard deviation (SD) from triplicate experiments. The production of amylase showed significantly higher activity ($p < 0.05$) compared to protease, indicating a strong potential for starch degradation applications.

The enzyme production data for both protease and amylase were collected from three independent experiments ($n = 3$), and the results were expressed as mean ± standard deviation (SD). The zone of clearance for each enzyme was measured in millimeters, indicating the enzymatic activity. Statistical analysis was performed using one-way analysis of variance (ANOVA) to determine whether there were significant differences in the production levels of protease and amylase.

The steps involved in the analysis are as follows:

- **Data Collection:** Three replicates of each enzyme production assay were conducted, and the diameters of the clearance zones (in mm) were recorded.
- The mean and standard deviation (SD) were calculated for the zones of clearance for both protease and amylase. For protease, the mean zone of clearance was 18.5 ± 0.8mm, while for amylase, it was 23.2 ± 1.1mm. Mean (x^{-}) = $\sum xi / n$ Standard Deviation (SD) = $\sum (xi - x^{-})2 / n - 1$

Discussion

In this study, Bacillus megaterium was successfully isolated from soil samples and characterized through morphological, biochemical, and molecular methods and also its solubilising index has also

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been determined. The study also evaluated the enzyme production capabilities of the isolate, focusing on protease and amylase. The findings provide insights into the potential applications of Bacillus megaterium in various industrial processes, especially in starch degradation.

Isolation and Identification

The successful isolation of Bacillus megaterium from soil highlights the prevalence of this bacterium in agricultural environments, where it plays a crucial role in nutrient cycling and plant growth promotion (Nannipieri et al., 2017). The large, rod-shaped, Gram-positive cells observed through microscopy, coupled with the colony morphology, are consistent with the characteristics reported for Bacillus megaterium in earlier studies (Kumar et al., 2013). The biochemical tests, particularly positive results for catalase, starch hydrolysis, and nitrate reduction, further support the identification of the isolate. These results align with the well-established biochemical profile of Bacillus megaterium, which is known for its metabolic versatility (Vary et al., 2007).

The molecular identification through 16S rRNA sequencing provided definitive confirmation of the isolate's identity. The high sequence similarity (99%) with other Bacillus megaterium strains from the NCBI database demonstrates the reliability of molecular techniques in bacterial identification. Moreover, phylogenetic analysis placed the isolate within the Bacillus megaterium clade, confirming its evolutionary relationship with other strains. This genetic similarity reinforces the findings from the morphological and biochemical analyses, indicating that the isolated strain belongs to Bacillus megaterium. The gene sequences has been deposited in DDBJ with Accession number LC510302.

Phosphate solubalization

Phosphate solubilization is a critical process for improving soil fertility and plant growth. Bacillus megaterium, as demonstrated in this study, is capable of solubilizing insoluble phosphate through the production of organic acids, such as gluconic acid, which lower the pH in its microenvironment, facilitating the dissolution of tricalcium phosphate in the soil (Choudhary et al., 2022). The solubilization index (SI) of 3.0 ± 0.1 observed in this study underscores the bacterium's efficiency in converting unavailable phosphorus into plant-accessible forms. These findings are consistent with previous research highlighting Bacillus megaterium's role in biofertilization and phosphorus mobilization (Goswami and Kalita, 2020). This ability to enhance phosphorus availability supports nutrient cycling in soil ecosystems, promoting sustainable agriculture by reducing reliance on chemical fertilizers. Synthetic phosphate fertilizers contribute to environmental issues, including water pollution and soil degradation, while microbial alternatives like Bacillus megaterium offer an eco-friendly and cost-effective solution (Jain and Sharma, 2020). Additionally, the bacterium's capacity for phosphate solubilization aligns with its broader application in biofertilization, where it also contributes to nitrogen fixation and production of phytohormones, further enhancing plant growth (Choudhary et al., 2022). The findings of this study highlight the industrial and agricultural potential of Bacillus megaterium as a biofertilizer, particularly in sustainable farming practices that aim to minimize environmental impact while maximizing crop productivity.

Enzyme Production

The enzyme production assays revealed that Bacillus megaterium exhibited significant protease and amylase activity. However, the production of amylase (23.2 ± 1.1 mm zone of clearance) was notably higher than that of protease (18.5 ± 0.8 mm zone of clearance), as confirmed by the statistical analysis ($p < 0.05$). These findings suggest that the isolated strain has considerable potential for industrial

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applications, particularly in processes involving starch degradation.Amylase production by Bacillus megaterium has been well-documented in literature, where its role in the breakdown of starch into sugars makes it valuable in industries such as food processing, textiles, and biofuel production (Gupta et al., 2003). The significant amylase activity observed in this study supports the utility of Bacillus megaterium as a source of amylase for biotechnological applications. Furthermore, the ability of Bacillus megaterium to produce protease highlights its potential use in detergent formulations, leather processing, and waste management, where protease enzymes are employed to degrade proteins (Rao et al., 1998).

Comparison with Previous Studies

The enzyme production levels observed in this study are consistent with earlier research on Bacillus megaterium. For example, Patel et al. (2016) reported similar zones of clearance for amylase production in their study of industrially relevant Bacillus species. Additionally, protease production by Bacillus megaterium has been reported in various studies, although the levels can vary depending on the strain and growth conditions (Kumar et al., 2012). The enzyme production potential of this isolate demonstrates its versatility and aligns with the broader characteristics of the Bacillus genus, known for its robust enzyme-producing capabilities.

Industrial and Environmental Relevance

The dual production of protease and amylase by Bacillus megaterium indicates its potential for diverse industrial applications. Amylase is widely used in the conversion of starch into simple sugars, a process essential in the production of ethanol, sweeteners, and bioplastics (Pandey et al., 2000). The high amylase activity observed in this study suggests that the isolated strain could be an efficient source of amylase for industrial biocatalysis, particularly in the biofuel and food industries. Similarly, proteases produced by Bacillus megaterium have applications in waste management, where they can break down proteins in industrial effluents, reducing environmental pollution (Joo et al., 2002).

Limitations and Future Prospects

While this study provides valuable insights into the enzyme production capabilities of Bacillus megaterium, further optimization of growth conditions, such as pH, temperature, and substrate concentration, could enhance enzyme yields. Additionally, the genetic manipulation of the isolate could be explored to increase its enzyme production capacity, as previous studies have shown that recombinant strains of Bacillus species can significantly improve enzyme activity (Schallmey et al., 2004). Future studies could also investigate the application of this strain in large-scale industrial processes, particularly in starch hydrolysis and protein degradation.

The results of this study demonstrate that Bacillus megaterium is a promising source of industrially relevant enzymes, particularly amylase and protease. The isolate’s ability to produce these enzymes in significant quantities suggests its potential application in industries such as food processing, biofuel production, and waste management. Further studies focusing on optimizing production conditions and Scaling Up The Process Will Help Unlock The Full Industrial Potential Of This Strain.

Conclusion

In this study, Bacillus megaterium was successfully isolated from soil and identified through a combination of morphological, biochemical, and molecular techniques. The findings highlight the versatility and industrial significance of Bacillus megaterium, particularly in the production of

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enzymes such as amylase and protease. The biochemical tests and 16S rRNA gene sequencing confirmed the identity of the isolate as Bacillus megaterium, while enzyme assays revealed significant amylase and protease activity, with amylase production being notably higher. The statistical analysis further validated the difference in enzyme production levels, with amylase showing significantly greater activity compared to protease. The ability of Bacillus megaterium to produce enzymes with industrial applications suggests that this bacterium could be a valuable resource for industries such as biofuel production, food processing, and waste management. The strong amylase activity, in particular, positions this strain as a potential candidate for processes involving starch degradation. The study demonstrated that Bacillus megaterium efficiently solubilized phosphate, achieving a solubilization index of 3.0 ± 0.1 on Pikovskaya's agar medium. This capability underscores its potential as a biofertilizer, enhancing soil fertility and promoting sustainable agricultural practices by improving phosphorus availability to plants. Future research should focus on optimizing growth conditions to enhance enzyme yields and exploring the genetic manipulation of this strain to maximize its industrial potential. Additionally, scaling up the enzyme production process for commercial applications will be an important step toward realizing the full biotechnological value of Bacillus megaterium.

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Application Diels-Alder Chemistry

Ajay M. Patil[1]*, Chandrashekhar G. Devkate[2], Uddhav Chaudhar[3], Shyam Takle[4]

[1]*Department of Chemistry, Pratishthan College Paithan, Chh.Sambhajinagar-431107, India
[2]Dept. of Chem.,Indraraj Arts, Com.and Sci.College, Sillod, Chh.Sambhajinagar-431112,India
[3]*Dep.ofChemistry,Kalikadevi Art's, Sci.&Comm.College, Shirur(Ka.),Dist.- Beed India
[4]Department of Chemistry, S.D.College Soegaon, Chh.Sambhajinagar-431107, India
* Correspondence: E-mail: patilam4@gmail.com

Abstract:-

The Diels–Alder reaction has long been established as an extremely useful procedure in the toolbox of natural product synthesis. It tolerates a wide spectrum of building blocks of different complexity and degrees of derivatization, and enables the formation of six- membered rings with well-defined stereochemistry. Now a days, many total syntheses of natural products have been reported that rely, at some point, on the use of a [4+2] cycloaddition step. The Diels–Alder reaction is one of the most popular transformations for organic chemists to generate molecular complexity efficiently. Surprisingly, little is known about its industrial application for the synthesis of pharmacologically active ingredients, agrochemicals, and flavors and fragrances. The Diels–Alder reaction has both enabled and shaped the art and science of total synthesis over the last few decades to an extent which, arguably, has yet to be eclipsed by any other transformation in the current synthetic repertoire. With myriad applications of this magnificent pericyclic reaction, often as a crucial element in elegant and programmed cascade sequences facilitating complex molecule construction, the Diels–Alder cycloaddition has afforded numerous and unparalleled solutions to a diverse range of synthetic puzzles provided by nature in the form of natural products. The selected application specially focus on large-scale applications from a process research and development perspective.

Keywords:- Diels-Alder, Cycloaddition, Click Chemistry, Nanomedicine

1. Introduction

After numerous near-discoveries of the [4+2] cycloaddition reaction by several luminaries in the field of organic chemistry during the early part of the 20th century [1, 2] the keen insight of Professor Otto Diels[3] and his student, Kurt Alder,[4] in properly identifying the products.

Up to the time of their receipt of the Nobel Prize in 1950 it seems that, for the most part, the synthetic community heeded the demand of Diels and Alder, as their cycloaddition reaction did not feature prominently in any total synthesis prior to the stereocontrolled generation of cantharidin [5] by Stork et al. in 1951, or the first synthesis of morphine [6] reported a few months later in which Gates and Tschudi employed the pericyclic process.

The apparent delay in applying the Diels-Alder reaction, or diene synthesis as it was known at the time, to total synthesis was likely the consequence of a variety of factors. First, with few exceptions, total synthesis during that period played a role inclined more towards structure verification than as its own unique vehicle to advance the field of organic synthesis, as it is practiced today. As such, in a discipline defined by converting known materials by existing methods into other compounds, practitioners would not likely have regarded being the first to employ a particular transformation in a synthesis as an important contribution, and the number of compounds in which the Diels-Alder reaction had been demonstrated was limiting in terms of potential synthetic targets. Moreover, the founders of the reaction, while they certainly made significant forays in terpene

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synthesis,[7] became diverted by other research concerns of greater interest to them, particularly in regard to understanding the mechanistic underpinnings of the reaction they had discovered.[8] Significantly, these efforts ultimately resulted in such important advances as the Alder endo rule that governs the stereochemical outcome of the typical Diels-Alder reaction.[9] The most dominant reason for the delay in the incorporation of the Diels-Alder cycloaddition into total synthesis, however, might be attributed to World War II and its aftermath, a period for which no analysis can properly estimate the challenges to conducting research in organic synthesis.

In this Chapter, we hope to highlight Application of Diels Alder reaction in the context of Synthesis having application in different area in organic synthesis. Our aspiration is that the delineated examples will sufficiently cover the various areas in which Diels-Alder methodology represents an indispensable tool for the art of total synthesis, and will reflect key paradigm shifts in the field through novel and inventive approaches to this classic reaction.

2. Application of Diels-Alder Reaction

The Diels-Alder reaction has been utilized in a wide array of biomedical and nano based applications due to its selective, tunable and reversibility properties. Examples of these include the use of Diels- Alder linkers as reversible conjugation points particularly in drug delivery and in the formation of self-assembled nanoparticles [10]

The Diels-Alder reaction has been described as a form of click chemistry, which is a class of chemistry which can proceed under mild simple conditions with little to no by-products and simple isolation procedures. Drugs and/or their components produced in this manner are highly sought after in drug development due to the ease of production and purification. In particularly the use of the Diels-Alder reaction is favoured, where all atoms of the reagents and product are retained. Typically, chemical reactions proceed with the formation of side products, which may require chemical scavengers or additives such as catalysers to promote the forward reaction. For example, the formation of water during an esterification reaction, requires the removal of water with dehydrating agents such as concentrated sulphuric acid. The atomic conservation property of the Diels-Alder reaction prevents the need for additives and catalysers to drive the reaction forward, which is an important advantage for biomedical applications where the purity of API's is paramount to efficacy.[11]

Nanomedicine is a relatively new field as a subgroup of nanotechnology. The scope of nanotechnology in medicine has focused on targeted drug delivery, wound healing, cancer treatment, and diagnostics including contrast agents to name a few[12] The advantageous properties of the Diels-Alder reaction have been exploited for furthering nanomedical research and developing biomedical applications.

The Diels-Alder reaction can be used in nanotechnology particularly in drug development and design due to its advantageous properties of atom conservation in both the forward and reverse reaction, the introduction of substituents unaffected by both reactions and the cycloadducts sensitivity to temperature. As such, Diels-Alder cycloadducts within drug development are often used as controllable labile linkers [13]. The use of controllable linkers is important as it confers control over payload release *in vivo*, rather than relying on physiological activity and/or time. Within the body, these linkers will therefore need to be chemically resistant to the physiological conditions they would be present in, such as the blood stream when intravenously injected. Breakdown of these linkers would also require conditions that do not adversely affect the patient such as elevated temperatures localised to tumours in the case of anti-cancer treatments [14].

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Even with all the potential advantages the Diels-Alder reaction highlights, there are several drawbacks that prevent the Diels-Alder reaction from having a wider range of industrial and medical uses. One drawback is the lack of enzyme mediated Diels-Alder reactions. Enzyme mediated synthesis of drug compounds and their precursors is gaining increasing interest due to their advantage of high selectivity for their substrates (reducing side reactions), reusability and eliminating the requirement for toxic chemical catalysts such as transition metals. Research is emerging for the development of man-made Diels-Alder enzymes (Diels-Alderase), in which the first was reported in 2010 by Siegal *et al*. [15]. This enzyme was designed by computationally determining the atomic orientation and shape of an active site required, for a Diels-Alder reaction between 4-carboxybenzyl *trans*-1,3- butadiene-1-carbamate and N,N-dimethylacrylamide. The enzyme was then synthesized in genetically modified *E. Coli* cultures. In comparison with metallic catalysts, the use of the Diels-Alderase, is an order of magnitude slower, but does produce cycloadducts with a higher stereoselectivity.

The Diels-Alder reaction is an excellent solution to the increasing demand for high speed, efficient "click" chemistry in the construction of larger repeatable polymers and dendrimers in mild conditions is already established and will likely support future synthetic efforts. This is evident in examples for both the forward and reverse reaction occurring at physiological temperatures in water without the need for UV radiation or catalysers, which is important for cell-friendly and biocompatible, click chemistry reactions.[16]

Tello and co-workers provides the possibility of developing microfluidics-produced iEDDA-crosslinked MPs as a potential drug vehicle and cell encapsulation system in the biomedical field[17].

The advent of the click chemistry paradigm has profoundly transformed the design of functional polymeric materials. Among the various reactions in the click chemistry toolkit, the inverse electron demand Diels–Alder (IEDDA) reaction is particularly notable for its rapid kinetics, high specificity, and bioorthogonality [18].

3. Conclusions and Future Perspectives

The numerous examples of the Diels-Alder reaction and applications described in these chapter are a small sample of the extensive research that has been birthed since its first description in 1928. A powerhouse in synthetic transformations that provides a plethora of chemical structures in which many are capable of efficient atomic conserving retrosynthetic reactions. With its highly established history in synthetic chemistry and other fields, there can be no doubt that the Diels-Alder reaction will continue to see an ever-expanding role in new synthetic enterprises, particularly in the field of synthetic chemistry, pharmaceutics, biomedical sciences, polymer and material sciences.

Finally, we offer the conjecture that Diels and Alder would be enormously pleased to know of the many important and elegant applications of their reaction in total synthesis. Indeed, they might even derive a considerable measure of satisfaction from the knowledge that their warning against the use of their reaction in total synthesis, a right they reserved for themselves alone, was not heeded by subsequent generations of chemists.

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Synthesis of isoxazole–carboxamide derivatives as melanoma and targeted nano-emulgel conjugate for improved cellular permeability

Kokane Balaji Digambar,
Department of Chemistry, Shri Kumarswami Mahavidyalaya, Ausa Dist.Latur (MS)

Abstract:

Cancer is one of the most dangerous and widespread diseases in the world today and it has risen to the position of the leading cause of death around the globe in the last few decades. Due to the inherent resistance of many types of cancer to conventional radiotherapy and chemotherapy, it is need to develop innovative anticancer medications. Recently, a strategy based on nanotechnology has been used to improve the effectiveness of both old and new cancer drugs.

Keywords: Nano-emulgel, ionic liquid, anticancer,isoxazole-carboxamide.

Objectives:

The present study aimed to design and synthesize a series of phenyl-isoxazole–Carboxamide derivatives, evaluate their anticancer properties, and improve the permeability of potent compounds into cancer cells by using a nano-emulgel strategy.

Experimental

The coupling reaction of aniline derivatives and isoxazole–Carboxylic acid was used to synthesize a series of isoxazole–Carboxamide derivatives. IR, HRMS, 1H-NMR, and 13C-NMR spectroscopy techniques, characterized all the synthesized compounds. The in-vitro cytotoxic evaluation was performed by using the MTS assay against seven cancer cell lines, including hepatocellular carcinoma (Hep3B and HepG2), cervical adenocarcinoma (HeLa), breast carcinoma (MCF-7), melanoma (B16F1), colorectal adenocarcinoma (Caco-2), and colon adenocarcinoma (Colo205), as well as human hepatic stellate (LX-2) in addition to the normal cell line (Hek293T). A nano-emulgel was developed for the most potent compound, using a self-emulsifying technique.

Results and discussion

The synthesis of novel 3-methyl-4-phenyl-isoxazole–Carboxamide derivatives (2a–2f) was presented in this paper. The coupling reaction to form the 3-methyl-4-phenyl-isoxazole–Carboxamide compounds (2a–2f) was afforded by using DMAP and ionic liquid (EAN) as activating agents solvent and catalysts, respectively. After 30 min, the afforded aniline derivative was added for each reaction [24], the mechanism of this coupling reaction by using the IL as activating agent is discussed in Scheme 1 [15, 26]. Then each reaction product was purified by column chromatography using different solvent systems (n-hexane, ethyl acetate, DCM, and ethyl acetate). The synthesis of these derivatives was confirmed by HRMS and all product masses matched the calculated masses. The yields of all final compounds were in the range of 59–81%, and these results yields seem very close to the previous literature with similar compounds and methods [18, 21]. The observed signals of 1H-NMR spectrums of the final products showed: firstly, a singlet signal for the proton of amide in ppm range of 9.20–10.78 for all compounds, secondly multiple signals in the aromatic area were observed, then a singlet signal integrated for 3 protons was observed around 2.62 ppm, that should be related to the CH3 group of Isoxazole ring. Moreover, the main observed signals of 13C-NMR spectrum showed a clear signal around 170 ppm that should belong to carbonyl carbone, various signals were

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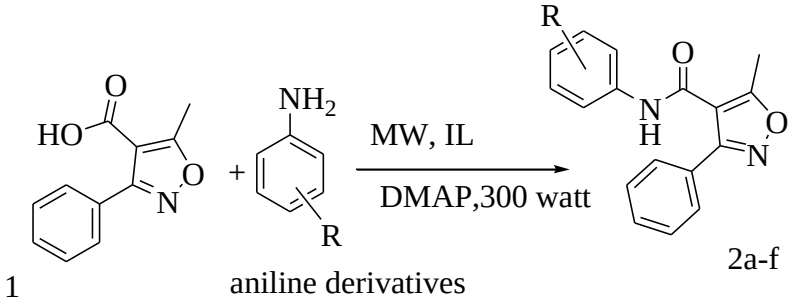
observed between 160 and 90 ppm for aromatic carbons as well signal around 12.4 ppm for aliphatic carbon CH3 of isoxazole ring.

Reaction scheme:



Biological activity:

To evaluate the antiproliferative activities of the synthesized compounds, the MTS assay was performed on B16-F1, Colo205, HepG2, Hep3B, CaCo-2, HeLa, and MCF7 cells, as well as the normal cell line, Hek293t. As shown in Table 2, seven concentrations were used (300, 100, 50, 10, 1, 0.5, 0.1 and 0.05 µM). Based on the results shown in Table 2, the compound 2a showed a broad range of activities on five cancer cell lines with an IC50 range of 7.54–129.17 µM, and this compound was the most potent structure against Colo205 and HepG2 cancer cell lines, with IC50 values of 9.179 and 7.55 µM, respectively, as well as potent on normal cell lines Hek293t with an IC50 of 2.54 µM. All of the synthesized compounds (2a–2f) showed potent to moderate activities against B16F1 with an IC50 range of 0.079–42.93 µM and the most active compound was the 2e compound. In contrast, our synthesized compounds showed weak or negligible activities against Hep3B, CaCo-2, HeLa, and MCF7 cancer cell lines.

Table 2.

IC_{50} (µM) of phenyl-isoxazole–Carboxamide compounds (**2a–2f**) on various cell lines

Code	2a	2b	2c	2d	2e	2f
R	2,5-Cl, 4-OMe	4-CF_3	4-(2-methoxy phenoxy)	2,5-SCH_3	4-NO_2	4-(thiophene)
Cell line B16F1	25.62 +	40.82	22.15	40.22	2.02	15.54
Colo205	10.12	192.34	233.23	78.20	162.45	123.56
HepG2	7.56	55.45	120.56	39.12	313.12	45.30
CaCo-2	130.12	213	345	256	334	344
HeLa	45.67	>200	>200	>200	>200	>200
MCF-7	>200	>200	>200	>200	>200	>200

Conclusion

The synthesized compounds 2a–2f showed different activities on B16-F1, Colo205, HepG2, Hep3B, CaCo-2, HeLa, and MCF7 cancer cell lines, ranging from moderate to potent activity compared with 5-FU and Dox anticancer drugs. The most potent compound, 2e, shows great activity

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on the B16-F1 cancer cell line, with an IC50 value very close to the Dox value (IC50 = 0.079 and 0.056 μM, respectively). To increase its activity on this cancer cell, a nano-emulgel was prepared to gain a fold effect, which improved from 79 to 39 nM in the nano form. The antifibrotic activities of the synthesized compounds at low concentrations were better than those of 5-FU. The synthesized compounds, especially in the nano form, could be a promising agent for melanoma cancer and further in vitro and in vivo studies should be conducted in the future.

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Physicochemical and Biological Studies of DHA Schiff Bases and Their Transition Metal Complexes.

[1]Heena K. Sayyed, Poonam D. Wawargire, Pratiksha N. Jagtap, Dhananjay G. Palke*
Department of Chemistry, Rajarshi Shahu Mahavidyalaya, Latur
(Autonomous)
Email: dhananjaygpalke29@gmail.com

Abstract:

The solid metal complexes of Cu (II), Ni (II), Fe (III) Co (II) Mn (II) and Cd(II) with DHA Schiff base ligand derived from 3,4-dimethoxy aniline were synthesized, characterized by elemental analysis, (FTIR, UV-VIS, 1HNMR and XRD) spectroscopic techniques, Thermal and Magnetic study. The antimicrobial (Anti-bacterial and Ant-fungal) activity of ligand and metal complexes have been screened in vitro against 1) Baccilus Subtilis 2) Staphyallococcus aureus 3) Aspergilus niger and 4) Candida albicans. The composition and structure of synthesized Schiff base ligand and all metal complexes confirmed by elemental analysis, (FTIR, 1HNMR, UV-VIS and Magnetic study) spectroscopic techniques, Stability of complexes confirmed by thermal study. The synthesized Schiff base ligand and all metal complexes are found to be biologically active. Co (II) and Cu (II) complexes exhibit maximum and Fe (III) complex exhibits minimum zone of inhibition.

Keywords: Dehydroacetic Acid, Schiff Bases, Metal Complexes, Biological Activity.

1. Introduction:

Dehydroacetic acid (3-acetyl-4-hydroxy-6-methyl-2H-pryan-2-one) and its derivatives are important class of compounds in organic synthesis, especially as starting materials for the preparation of various heterocyclic systems viz. Schiff bases, Mannich bases, Chalcone etc. Schiff bases are one of the most widely used as chelating ligands in co-ordination chemistry. In the 21st century, coordination chemistry becomes the important area of research in inorganic chemistry. It is a rapid developing branch of chemistry due to large applications in the field of organic synthesis, asymmetric synthesis, catalysis, as bleaching agents, industries, dyes, drugs. The metal complexes are applied in medicinal, analytical and diagnostic purposes in the living system. Because of magnetic and radioactive properties they are used in optical images, Magnetic Resonance Imaging (MRI). Schiff bases and their metal complexes can catalyze the reactions, show biological activities such as antimicrobial, antifungal, antiviral, synergistic, antioxidant, anti-inflammatory, analgesic, antitumor, cytotoxic, antidiabetic, anti-fertility, [1,2] anti-tumor activity [3] DNA Photoclevage activity [4] etc.

Popova and Berova reported that copper complexes are good for a liver function and its level in blood and urine has an influence in a pregnancy disorder, Nephritis Hepatitis, Leukemia, Leprosy, and Anemia in children.[5]. Here in we describe the synthesis and characterization of the Schiff base derived from Dehydroacetic acid and 2-aminopyridine. The metal complexes of Cu (II), Ni (II), Fe (III) and Co (II) Mn (II), and Cd (II) were synthesized. The Schiff base and metal complexes are characterized by elemental analysis, (FTIR, UV-VIS, 1HNMR and XRD) spectroscopic techniques, Thermal and Magnetic study.

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2.Experimental Details:

Dehydroacetic acid for synthesis was purchased from E-Merck Germany, 3, 4-dimethoxy aniline AR grade from Loba chemie Pvt. Ltd are used for synthesis of Schiff bases. AR grade metal chlorides E-Merck and Loba chemie Pvt. Ltd were used for synthesis of metal complexes. The solvents were dried distilled before use following procedure [6]. The C, H and N analysis were obtained from Perkins Elmer CHN Analyzer (2400).The IR spectra of ligand and the metal complexes were recorded on alpha Brucker FTIR spectrophotometer in the range 4000-400 cm-1. The electronic spectral measurements were made on Shimandzu UV –VISIBLE Spectrophotometer UV 160. Research centre Dept. of Chemistry Rajarshi Shahu Mahavidyalaya, Latur (MS). The 1HNMR spectrum of ligand is recorded on Brucker FT-500 MHz NMR Spectrophotometer in CDCl3 by using solvent TMS as reference substance. X-Ray analysis at central instrumentation centre, Solapur University, Solapur. TGA -DTA scanning at Central Instrumentation Centre, Savitribai Phule University, Pune. Antimicrobial activity tested from Research centre Department of Biotechnology R. S. M. Latur.

3.Synthesis of Schiff Bases:

DHA Schiff Bases are synthesized by using standard procedure [7,8] by which the equimolar solutions of Dehydroacetic acid (0.01mol) and 3, 4-dimethoxy aniline (0.01mol) were dissolved in 25 ml of dry ethanol taken in round bottomed flask .the content of flask refluxed for four to six hour on 1 RML rotamantle with magnetic stirrer. Upon cooling the light yellow colored solid mass of Schiff base that separated out was filtered, washed, with a small portion of ethanol and dried. A pure product was obtained by recrystallisation from ethanol and drying in vacuum desiccators the purity of product was ascertained by TLC and melting point.

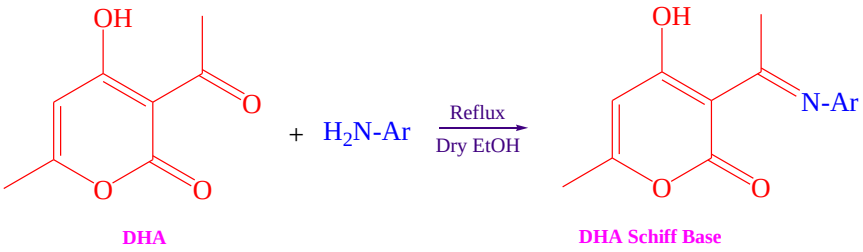

Fig.01: Synthesis of Schiff base

Synthesis of Metal Complexes:

Methanolic solution (0.002 mol) of DHA Schiff bases derived from 3,4dimethoxy aniline refluxing with methanolic solution(.001 mol) of metal chloride in 2:1 molar ratio yielded metal complexes after the addition of 10% methanolic solution of ammonia.[8]

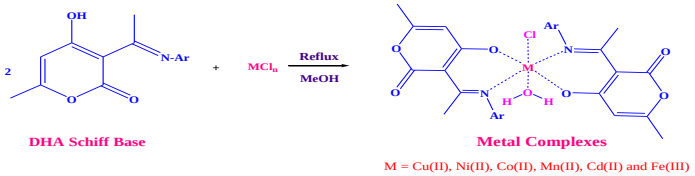

Fig.02: Synthesis of Metal Complexes.

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Results and discussion:

Synthesized Schiff base is yellowish colored solid stable to air, non-hygroscopic, insoluble in water and soluble in hot alcohols. All the metal complexes were colored solids, stable to air non-hygroscopic. They were insoluble in water, methanol, ethanol, but soluble in DMF and DMSO. The melting points of ligand and metal complexes were determined by open capillaries. The analytical data is shown in Table 1.

Compounds	Color	F. Wt.	M. P. °C	Found (calculated) %				
				C	H	N	M	Cl
$C_{16}H_{17}NO_5$	Yelowish	303	115	63.43 (63.7)	5.62 (5.61)	4.70 (4.62)	--------	----------
Cu (II) DL	Greenish	776	295	48.88 (49.48)	04.11 (04.38)	03.05 (03.60)	08.42 (08.18)	09.20 (09.14)
Ni (II) DL	Orange	735.7	>291	51.96 (52.19)	04.41 (04.62)	03.57 (03.80)	07.43 (07.99)	09.62 (09.65)
Fe (III) DL	Reddish	768.21	287	49.13 (49.98)	04.19 (04.42)	03.21 (03.64)	07.35 (07.26)	09.18 (09.24)
Co (II) DL	Pink	843.93	>300	44.32 (45.50)	03.63 (04.02)	03.43 (03.31)	06.31 (06.98)	08.48 (08.41)
Mn (II) DL	Yellowish	803.9	288	46.85 (47.76)	04.08 (04.22)	03.23 (03.48)	06.40 (06.83)	08.64 (08.83)
Cd (II) DL	Yellowish	972.92	>300	39.72 (39.46)	03.12 (03.49)	03.07 (02.87)	--	---

1H-NMR:

The 1HNMR spectra of ligand in CDCl3 at laboratory temperature showed the signals at δ (ppm) values for DL ligand 2.15 (3H, s, C6 – CH3) , 15.7 highly downfield (1H, s ,O-H) , 5.78 (1H, s, C5-H) , 2.6 (3H, s, N=C-CH3) methyl hydrogen linked carbon azomethine, for DHA moiety[7] 3.94 (6H,s, two Ar O-CH3), 7.3 (1H,s,C2 of Ar), 6.65-6.95 (2H,m,C5 & C6) aniline moiety.

IR Spectra:

The IR spectrum of free ligand shows a broad weak band at 3238 cm-1 which is due to intra molecular hydrogen bonding between enolic O-H and N of azomethine. The band at 1685 cm-1 assigned to ν (C=O) lactone carbonyl , 1639 cm-1 to ν (>C=N) (azomethine) , 1388 cm-1 to ν (C-N) aryl azomethine and 1236 cm-1 to ν (C-O) enolic group. The disappearance of broad weak band at 3238 cm-1 in the IR spectra of complexes indicate the deprotonation of enolic oxygen which is supported by and the upward shift in ν (C-O). The downward shift in ν (C=N) azomethine during coordination to the metal ion.[3,4] It is further supported by and the upward shift in ν(C-N) azomethine which indicate the participation of azomethine N and enolic O in the complex formation.

The IR Spectra of the metal complexes showed a new band at 650-540 and 580-450 cm-1region which can be assigned to ν (M-O) & ν (M-N) vibrations.[5,6] The characteristic IR frequencies of the ligand and metal complexes are shown in Table 2.

Table 2: Characteristic IR Frequencies (cm^{-1}) of the Ligand and Metal Complexes.

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Compounds	ν(C=O)	ν(C=C)	ν(C=N)	ν(C-N)	ν(C-O)	ν(M-O)	ν(M-N)
L	1685	1578	1639	1388	1236	----------	----------
Cu(II) L	1698	1574	1632	1384	1319	562	479
Ni(II) L	1704	1584	1630	1390	1325	556	465
Fe(III) L	1709	1580	1641	1397	1241	527	460
CO(II) L	1692	1576	1624	1389	1258	561	477
Mn(II) L	1700	1577	1615	1395	1256	624	473
Cd(II) L	1705	1573	1629	1387	1321	564	473

Magnetic measurement and electronic absorption spectra:

The electronic spectra of the Cu (II) complexes in DMSO shows the band at 11257-16444 cm-1 for ligand D L assignable to 2Eg¬> 2T2g transition which is characteristic of octahedral geometry [11]. This further supported by magnetic moment values (1.78μB) within the required range for d9-system [12]. The electronic spectra of the Ni (II)-DL complex shows three bands in range 10734(v1), 15245(v2) and 23733(v3) assigned to the transitions 3A2g(F) ¬>3T2g and a charge transfer transition, respectively, suggesting octahedral geometry of the complexes. [13] The electronic absorption spectrum of Co (II) complexes had three bands in range 12438 (v1), 18567(v2) and 27477 (v3) which may be attributed to three spin-allowed transitions 4T1g (F) ->4T2g(F), 4T1g (F) ¬>4A2g(F) and 4T1g (F) ¬>4T2g(P), respectively, suggesting an octahedral geometry. The effective magnetic moment values (4.42μB) were found to be well within the range as expected for octahedral geometry [14]. The electronic spectra Mn(II) complex showed two bands at 17682 cm-1 (v1) and 23212 cm-1 (v2) assigned to transition 6A1g¬> 4T1g and 6A1g ¬>4T2g, respectively, indicating octahedral geometry. The magnetic moment value (5.05 μB) which is slightly lower than the spin only value expected for octahedral Mn (II) complexes [15]. This may be due to the presence of magnetic exchange and small traces of Mn(II) species. The electronic spectra of the Fe (III) complexes showed three bands at 16254 (v1), 22685 (v2) and 29578 cm-1 (v3) assigned to transitions 6A1g¬>4T1g(D), 6A1g¬>4T1g and 6A1g¬>4T1g, respectively and the magnetic moment values (5.58 μB) suggesting high spin octahedral geometry[16, 17]. The Cd complex is diamagnetic. The magnetic and electronic spectral data is relevance for the proposed structure of complexes shown in Table-3.

Table 3: Magnetic and electronic absorption spectral data (in DMSO) of the complex

Compound	μ_{eff}	ν(cm^{-1})	Geometry
Cu(II) L_1	1.78	1125 and16444	Octahedral
Ni(II) L_1	2.84	10734, 15245 and 23733	Octahedral
Fe(III) L_1	5.58	16254, 22685 and 29578	Octahedral
CO(II) L_1	4.42	12438,18567 and 27477	Octahedral
Mn(II) L_1	5.05	17682 and 23212	Octahedral

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Cd(II) L_1	1.72	-------	Octahedral

Thermo Analytical Techniques:

There is no mass loss up to 200°C indicating the absence of lattice and coordinated water in the TG curve of Ni (II)-DL metal complex and exhibit high initial thermal stability. The TG thermo gram shows a first step decomposition in the range of 200-450°C with mass loss 39.00% and the corresponding exothermic peaks at 190°C and 375°C in DTA curve specify the decomposition of non-coordinated part of ligand in a relatively fast but moderate oxidation process. The second step of decomposition is occurs in the range of temperature 500-700°C with a further mass loss of next 52.00 % indicates the decomposition of the coordinated part of a ligand of the complex through a slow process. The organic part decomposes in the range 500-700°C that is also shown by broad exotherms in this range in DTA curve. Finally, the residue of Nickel oxide remains at 730°C.[18]

XRD Powder Diffraction:

The powder X ray diffraction of Fe (III) complexes of ligand DL was screened in the range 10 to 850 at wavelength λ 1.543 The diffractogram and associated data depict the data 2θ values of each peak relative intensity and inter planer spacing (d-values). The diffractogram of Fe (III)-DL complex had 14 reflections with maxima at 2θ 12.86 0 and 13.580 corresponding to d value 7.8775 and 6.5144. The X ray diffraction pattern of these complexes with respect to major peak of relative intensity greater than 10% has been indexed by using computer program. The above indexing method also yields Miller indices (h k l) unit cell parameter and unit cell volume. The unit cell of Fe (III)-DL complex yielded values of lattice constant a = 24.7804( ) , b = 7.5468( ) c -= 24.778( ) and unit cell volume V =624.8758( ) 3. α = ϒ = 900 and β = 103.32º required for sample to be Crystal system Monoclinic and Lattice Type P found to be satisfactory.[19]

Antibacterial and Antifungal Activity: The antimicrobial potentiality of DHA Schiff base ligands and their metal complexes was carried out by the agar well diffusion method [20]. The minimum inhibitory concentration of DHA Schiff base ligands and their metal complexes was determined by adopting the standard procedure of the National Committee for Clinical Laboratory standard (2004).[21] In vitro antibacterial and antifungal activity was screened by considering zone of inhibition of growth. The synthesized Schiff base L and its metal complexes were screened with their different concentrations with standard antibiotics such as streptomycin (1 mg/mL) and griseofluvin (1 mg/mL). DHA Schiff base ligand weak anti bacterial but shows strong antifungal activity. Antibacterial activity significantly increases on coordination because coordination reduces the polarity of metal ion due to partial sharing of positive charge with ligands that increase the lipophilic nature of metal ion in complex.[4, 22]This enhanced antimicrobial activity of metal complexes is because of the lipophilic nature of metal ion in complex.[23] The Antimicrobial activity data is presented in Table 4 and Fig.4 .

Table 4: Antibacterial and Antifungal Activities Data.

Sample	*B. subtilis*^{m}	*S. aureus*^{m}	*A. niger*^{m}	*C. albicans*^{m}
DL	18	11	10	16
Cu(II)-DL	21	17	14	13
Ni(II)-DL	8	12	12	14
Fe(III)-DL	6	5	11	12

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Co(II)-DL	21	16	22	19
Mn(II)-DL	9	13	14	15
Cd(II)-DL	11	12	14	16
Streptomycin	16	19.5	0	0
Griseofulvin	0	0	25	22

m=Zone of inhibition in mm.

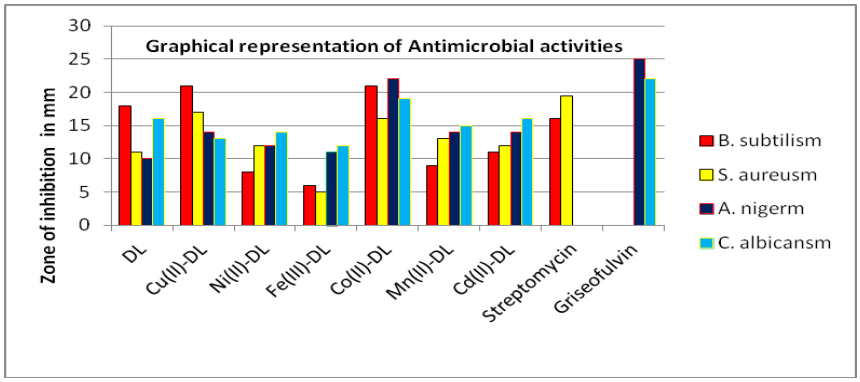

Fig.04: Graphical presentation of antibacterial and antifungal activities.

Conclusion:

Composition of Schiff base and metal complexes confirmed by elemental analysis. Structure of Schiff base and metal complexes confirmed by IR and 1H-NMR study, magnetic susceptibility measurement of and electronic spectral data of the complexes suggest the octahedral geometry. Thermal study shows thermal stability, and X- Ray diffraction studies concluded that all transition metal complexes synthesized having monoclinic crystal structure and P lattice type. DHA Schiff base ligand exhibits weak activity against bacteria but shows strong antifungal activity. Antibacterial activity significantly increases on coordination due to increase in lipophilic nature of metal ion in complex. Co (II) and Cu (II) complexes exhibited maximum zone of inhibition while Fe (III) complex exhibited minimum zone of inhibition.

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Acoustical study on copolymer as well as terpolymer resulting from same monomers.

Smita .S.Kharkale,-Bhuyar
[1]Department of chemistry, Shri Lemdeo Patil Mahavidyalaya, Mandhal, Nagpur,Maharashtra,India
Email: smitakharkale2013@gmail.com

ABSTRACTS:

The copolymer have been synthesized by condensation of p-hydroxy benzoic acid and formaldehyde in 2 molar HCl. The terpolymer have been synthesized by condensation of p-hydroxy benzoic acid urea and formaldehyde in 2 molar HCl Density ultrasonic velocity and viscosity of terpolymer and copolymer have been measured in N,N DMF at 283K,288K,293K,298K and303K.The acoustic impedance, adiabatic compressibility ,intermolecular free length etc have been calculated from the experimental data. The results are discussed in the light of solute-solvent interaction and structural effects on the solvent in solution.

***Keywords*:** Terpolymer, copolymer, acoustic impedance, adiabatic compressibility, intermolecular free length, viscous relaxation time.

1.Introduction:

Ultrasonic waves have acquired the status of an important probe for the study of structure and properties of matter [1].In basic science, these waves are used to provide information on the behavior of microscopic particle of matter [2].Through the higher order elastic constants involved in the propagation of these, an insight into the interaction in solid is obtained. The absorption and dispersion of waves provide information about relaxation processes in liquid [3]. The study of molecular interaction in liquids provide valuable information regarding internal structure, internal pressure ,molecular association, complex formation etc.The various experimental techniques available to study them are NMR,microwave,ultraviolet and infrared spectroscopy and ultrsonics.While NMR technique reflects the effect on the proton bearing molecules. The microwave absorption provides information through the dielectric constant, neutron and X-ray scattering, helps in the study of molecular motion. The spectroscopic techniques provide useful information on intermolecular interactions cannot be resolved from the observed spectra. The ultrasonic techniques on the hand reveal weak interactions due to its useful wavelength range. Ultrasonic parameters are directly related to a large number of molecular and thermodynamic parameters.

The ultrasonic velocity and absorption coefficient measurement have furnished method for studying molecular and structural properties of fluid. There exists close relationship between the ultrasonic velocity and chemical or structural characteristics of molecules of fluid. This gives a property of basic importance to sound velocity in molecular theory of fluid. Sound velocity is a thermodynamic function.Many other thermodynamic properties of electrolyte solutions are determined from sound velocity. In recent years ultrasonic velocity studies in many of the aqueous [1-2], pure non-aqueous [3-4] and mixed [5-10] electrolytic solutions have led to new insights into the process of ion and ion-solvent interactions. In the present investigation, free intermolecular length acoustic impedance, adiabatic compressibility, viscous relaxation time of copolymer derived from p-hydroxy benzoic acid and formaldehyde and terpolymer derived from p-hydroxy benzoic acid, urea

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and formaldehyde in N, N,DMF has been evaluated at different temperatures over range of concentration using experimentally determined values of viscosity, density and ultrasonic velocity.

2. Experimental:

The chemicals used were of analytical grade. They were obtained from E. Merck chemical company. All reagents were used after purification by fractional distillation. The compounds were prepared in the laboratory [4]. Densities, viscosities, and velocities were measured at different temperatures. The temperature was maintained constant by a thermostatically controlled water bath LTB-10. The densities were measured by the hydrostatic plunger method. A cell was designed and fabricated specially for this purpose. A small glass tube of length 3.2cm and diameter 0.7cm sealed with a glass hook at the upper end and filled with mercury was used as plunger. A monopan digital balance of least count 0.0001gm was used to record change in plunger weight dipped in solutions correct to fourth decimal place.. The viscometer was calibrated with doubly distilled water and N, N, DMF. Care was taken to reduce evaporation during the measurements. A thoroughly cleaned and dried Ostwald viscometer filled with experimental liquid was placed vertically in a glass-fronted, well-stirred water bath. After thermal stability was attained, the flow times of the liquids were recorded with an accurate stopwatch correct to (0.01 s). The present values of viscosity for the various liquids agree with the literature values within a deviation of the order of (0.01poise) Ultrasonic sound velocity measurement were made by variable path single crystal interferometer (Mittal Enterprises, Model F – 81S) at 2 MHz with accuracy of ± 0.03%.

3. Results And Discussion:

Different thermodynamic parameters such as intermolecular free length (Lf), specific acoustic impedance (z) and relative association (RA) [28] Viscous relaxation time (τ),adiabatic compressibility(βs) have been calculated from at 283K.288K,293K,298K and 303K,using ultrasonic velocity(U) ,viscosity(η) and density(ρ) of these solutions with the help of the standard equations to have an insight on ion-and ion-solvent interactions.

$$Lf = K \times \sqrt{\beta s} \qquad \ldots\ldots\ldots (1)$$

$$Z = Us \times ds \qquad \ldots\ldots\ldots (2)$$

$$R_A = \frac{\rho s}{\rho o}\left(\frac{Uo}{Us}\right)^{1/3} \qquad \ldots\ldots\ldots (3)$$

$$T = 4\eta / 3\rho s Us^2 \qquad \ldots\ldots\ldots (4)$$

$$Bs = U^2\rho^{-1} \qquad \ldots\ldots\ldots (5)$$

Where ρs, ρo,η,Us,Uo are the density of solution, solvent, viscosity velocity of solution and solvent respectively. K is Jacobson constant. The experimental data of ultrasonic velocity(Us),density(ρs),viscosity(η) of copolymer and terpolymer in N,N,DMF is given in table 1.For both the polymers ultrasonic velocity(Us),density(ρs),viscosity(η) increases with concentration. Various acoustical parameters were evaluated from experimental data of ultrasonic velocity (Us), density (ρs), viscosity (η) using the above standard equations. These parameters are given in table 2. The ultrasonic velocity (Us) depends on intermolecular free length (Lf).The ultrasonic velocity (Us) increases with decrease in Lf. For both the polymers Lf decreases with concentrations which suggest the presence of solute-solvent interactions. This is further confirmed by viscosity values which increase with increasing concentration suggesting more association between solute and solvent

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molecules. The adiabatic compressibility (βs) and viscous relaxation time (τ) are also observed to decrease with increasing concentration for both the polymers which further confirms the presence of solute-solvent interactions. The variation of Acoustic impedance with concentration is given in the table3.From the data, it is evident that Z values increases with increase in concentration of polymer. This is in agreement with the theoretical requirements as Us and ρs both increase with increase of concentration of solute in solution. The increase of Z values with solute concentration can be attributed to the effective solute-solvent interactions. The viscosity also increases with increasing concentration of solute in solution. This indicates the solute-solvent interaction. It is a measure of cohesiveness or rigidity present in between either ions or ion-solvent or solvent-solvent molecules present in a solvent or solution. In both the polymers all the parameters shows the same variations but in case of terpolymer the values are higher which suggest that as compared to copolymer the solute-solvent interaction is stronger in terpolymer. This may be due to the presence of third monomer that is urea which makes the structure of polymer more rigid thereby increasing the interactions.

Experimental results reveal that ultrasonic velocity with the temperature.Decrese in ultrasonic velocity may be attributed to solute-solvent interactions. It is observed that the value of βs increases with the temperature. This may be due to the presence of solvent molecules around the ions. It could be seen from Table 1 that the intermolecular free length (Lf) increases with the temperature, which reveals that there is a weak solute-solvent interactions as the temperature increases. This may also imply that the increase in number of free ions, showing the occurrence of ionic dissociation due to weak ion-ion interactions.

The acoustic impedance Z decreases with increase in temperature. This also suggests that as the temperature increases the interaction decreases. In both the polymers the trends are same but in case of terpolymer all the parameters show higher value which shows that the solute-solvent Interactions Is More In Terpolymer.

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Synthesis of Preservative and its application in Gel formation

Aakash S. Singare[1], Sana[2] Gadiwan, Bhagwan R. Patil[3], Seema G. Mehatre[4], Nanda S. Korde*
[1]School of Chemical Sciences, S.R.T.M.University, Nanded
[2,*] Dayanand Science college, Latur
[3]Sharda Mahavidyalaya, Parbhani
[4]Shri Chhatrapati Shahu Maharaj Sainiki Junior college, Udgir

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Abstract: Oftenally in herbal medicine Aloe vera, known as Curaçao Aloe or Barbados,. The Aloe vera plant acted as medicine in Ayurvedic, Homoeopathic and Allopathic.The leaves of aloevera contains numerous amino acids, natural sugars vitamins, enzymes and minerals etc. It shows purgative, antimicrobial, anti-inflammatory, anti-oxidant, aphrodisiac, anti-helminthic, antifungal, most of cosmetic values and antiseptic activity. Aloevera juice has potential to cure sunburns, burns, minor cuts, acne, skin cancer and it gives glowing youthful skin.According to ayurvedic literature, for the treatment of various diseases such as fever, colic, indigestion, worm infestation, splenomegaly, liver disorder aloevera is applicable. Also it is used as powerful detoxifier and immune-booster.
Keywords: Aloevera, citric acid, healthy and beauty skin

1. Introduction

Aloevera is a cactus like plant that rows in hot and dry climate. In Trinidad and Tobago, aloe vera gel is utilized as an ethnomedicine. For the treatment of burn wounds and in the healing process, reduce inflammation, and tissue scaring ,aloevera has been used commomnly.[1]

Due to medicinal and cosmetic (skin care) properties, Aloe vera plant has been used from centuries. It has Kumari , Ambudisrava or Vipulasrava, Maata, GhritaKumarika, Deerghapatrika, Amara or Ajara, Grihakanya, Sthuladala, Gandala, Kanya, MriduKanya, Sthaleruha, Bahupatra, Kantakapravruta, Veera, Bhringeshta, Vranaghni, Taruni, Rama, Kapila and Sukantaka are the *Sanskrit* synonyms [2]. Aloe vera plant classified as follows: Kingdom: Plantae, Family: Asphodelaceae, Genus: Aloe, Species: Aloe vera ,. Order: Asparagales, Andalso, there are a number of synonyms; Aloe barbadensis Mill, Aloe indica Royle, Aloe perfoliat Linn. var Vera and Aloe vulgaris Lam.[3] Most of the Aloe plants are not toxic, but a few are extremely poisonous. Aloe vera gel is applied with only a few allergic reactions being reported.[5] The productiveness of aloevera gel to treat burn wounds, genital herpes, and seborrhea dermatitis have been shown effectively. For the treatment of type 2 diabetes, the other indications such as psoriasis or internal implementations remain indecisive. The major solicitation of aloe vera gel as a skin moisturizer in cosmetics has proven its fruitfulness and as an après treatment for sunburnt and suntanned. Aloevera plant is a stemless or very short stemmed. In summer the flowers of aloevera produced. Flower being pendulous, with a yellow tubular corolla which is 2 – 3cm long. [6, 7] It is believed that the origin of the Aloe vera is Arabia, Somalia, or Sudan and a recently discovered in Oman.[8] At present, Aloevera plant is spread throughout the tropics and subtropics in dry regions. in the Asia , America, and Australia). As a cultivated plant, it is probably present in all countries of Africa.[9]

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Description: The colour of leaves of aloevera plant is green to grayish. Aloevera gel was obtained by slicing the leaf of the plant. The gel should be free of yellow coloured parts present in leaf. The gel is clear, odorless, and tasteless.

2.Experimental

Materials: Sodium hydroxide (NaOH), calcium chloride ($CaCl_2$), lemon juice, sulphuric acid (H_2SO_4) , fresh aloe juice, Agar-Agar powder, Vit-C (500mg), Sandalwood Oil, Almond Oil etc were used for this preparation.

Experimental methods:

1) Synthesis of Preservative:

- 50ml lemon juice extracted from the lemon juice and then filtered it.
- In 60ml distilled water, 8g NaOH was dissolved.
- Also prepared solution of 10g $CaCl_2$ in 60ml distilled water.
- NaOH solution and $CaCl_2$ solution were added in lemon juice.
- After this addition, calcium citrate precipitate was obtained then filtered and collected the precipitate.
- 100ml dil. H_2SO_4 was added in precipitate and stirred vigorously.
- Filtered the solution and heated for 2-3hours.
- Cooled the solution in ice cold water for 24hours, crystals were separate out. Filtered it and dried it.
- Recrystallised in alcohol.

Mp:152,

FTIR spectra of citric acid crystals revealed major peaks at 3310, 2618, 1728, and 1208 cm^{-1} depicts stretching of -OH, C-H, C-C, and C=O respectively. A peak at 3310 cm^{-1} represents the presence of moisture.[10] The peaks at 2618, 1728 and 1208 cm^{-1} represent the vibrational motions of functional group stretching in citric acid molecule.[11] However, the characteristic absorption band at 1285 cm^{-1} corresponds to the CH_2 stretching vibration in citric acid crystals.

2) Synthesis of gel:

1) Fresh aloevera leaf was taken. Washed it with water to remove oil dirt & dried it with clean cotton cloth.
2) Cut the leaf in equal part & collected the pulp in container.
3) Using mixer grinder, converts the aloevera pulp into juice (liquid).
4) Filtered the juice and heated for 2-3 min to remove the remaining pulp by maintaining the temperature 50-60°c.
5) 1 g citric acid (gelating agent) was added in 20 ml water in beaker and stirred till it completely dissolved in water.
6) Boiled this beaker for few minutes & further immediately transferred the 30 ml juice into hot solution of agar-agar.
7) Then 500mg vitamin-C , 2ml almond oil &2-3 drops of sandalwood oil were added & stirred continuously for 10-12 minutes . Further added food grade (Green Colour) into a gel.
8) Cooled the liquid at room temp then liquid was converted into gel.

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Mechanism of Action:

1. Effects on skin exposure to UV and gamma radiation: UV radiation from sunlight produces ozone in the stratosphere and can cause a variety of health issues. Such as skin cancer, mutation in DNA and suppress the immune system's response to new skin cells, eye damage, premature aging. Gamma radiation dare ionizing radiations and hazardous to life. They can cause tumours, dradiation sickness. They can destruct bone marrow and internal organs because of their high penetration power. But Aloe vera gel has been reported to have a protective effect against these radiation

2. Moisturizing and anti-aging effect: Mucopolysaccharides present in aloevera gel helps in binding moisture into the skin. Aloevera produces the collagen and elastin fibers due to which the skin becomes more elastic and less wrinkle.

3. Antiseptic effect: Many antiseptic agents such as Lupeol, salicylic acid, urea nitrogen, cinnamonic acid, phenols and sulfur are present in aloevera and these antisepting agents showed inhibitory action on fungi, bacteria and viruses.

4. Healing properties: Aloevera gel increased collagen content of the wound as well as also changed collagen composition and enlarged the degree of collagen cross linking. Due to this, it quicken wound contraction and enlarged the breaking strength of resulting scar tissue.

Evaluation of herbal aloe-vera gel

1. Absorption test

Absorption test was done by applying through gel on to the skin and rubbed until it gets completely absorbed.

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2.Skin Irritancy test

This test was done by applying a prepared aloevera gel on hand's back skin and leave it for 15 minutes to check irritation reaction such as swelling, ,itching and redness effect on the skin.

3.pH test

The pH value of this prepared herbal Aloe-vera gel were determined by using digital pH meter, **4. Smoothness**

The smoothness of the prepared gel was assessed through touch examination , by rubbing the gel between their fingers and made observations regarding its texture. We recorded whether the gel felt smooth, clumped, homogeneous, or harsh.

Conclusion:

In this research work we have synthesized citric acid and used as preservative in alorvera gel formation. It seems that the application of citric acid in aloevera gel formation can improve skin health. It gives healthy and bright skin. Aloevera, as a supportive treatment along with current method, can enhance wound healing and promote the health. Promisingly it may also provide other health benefits, largely due to its antioxidants property.

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$CoFe_2O_4$ Nanoparticles with Cr^{3+} Substitution: Structure, Morphology, Cation Distribution and Magnetic Properties

Vishnu S. Shinde
Shri Chhatrapati Shivaji College, Omerga Dist. Dharashiv (MS)-413 606
Email- drvishnushinde**@gmail.com**

Abstract

The present investigations deal with the effect of trivalent chromium ions (Cr^{3+}) on structural and magnetic properties of nanocrystalline cobalt ferrite ($CoFe_2O_4$) nanoparticles. The samples of $CoCr_xFe_{2-x}O_4$ (where x = 0.0 to 1.0 in step of 0.2) were successfully synthesized by citric acid-assisted sol-gel auto combustion method. Further, the prepared samples were characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), and infrared spectroscopy (IR) and pulsed field hysteresis loop technique for structural, morphological and magnetic properties analysis, respectively. XRD patterns showed the formation of single-phase cubic spinel structure with broad Bragg's peak for all the samples. The value of lattice parameter was found to be decreased with chromium substitution x. Cation distribution studies revealed that Co^{2+} and Fe^{3+} occupied both A and B sites, whereas Cr^{3+} ions occupied only B site. SEM analysis of the prepared samples confirmed the nanocrystalline nature of the material. The two absorption bands belonging to spinel structure were observed in IR spectra. Saturation magnetization (MS), remanence magnetization (Mr) and coercivity (HC) was found to be decreased with increase in chromium substitution x.

Keywords Cr^{3+} substitution · $CoFe_2O_4$ nanoparticles · XRD · Cation distribution · M-H curve

1 Introduction

Spinel ferrites basically recognized by the formula MFe_2O_4 (where M is divalent metal ion) have become the most requisite potential materials for technological perspective in a broad range of frequency ranging from microwave to radio frequency (RF) [1, 2]. The main advantage of spinel ferrite materials is the enormous compositional variability by the substitution of diverse cations in the parent crystal structure (i.e. at the tetrahedral and octahedral sublattices) and this disparity in cation distribution modifies many physical pro- perties of spinel ferrites such as raise in DC resistivity, low dielectric losses and necessary magnetic character [3, 4]. Recently, investigations on nano-sized spinel ferrite particles have attracted substantial concentration for their various physical and chemical properties, which are strikingly different from those of their bulk counterpart [5]. Magnetic properties of spinel ferrite nanoparticles have been intensively studied and the mechanism of the size effect is generally well understood in terms of the magnetically inactive surface layer [6]. In case of mixed spinel ferrite nanoparticles, the magnetization and other magnetic properties are affected through the influence of small size [7]. The magnetic properties of the spinel ferrite materials originate from the anti-ferromagnetic coupling between two sublattices namely octahedral [B] and tetrahedral (A) sublattices. The net magnetization of spinel ferrite nanoparticles results from the difference between these two sublattices (A and B) [8]. In the family of spinel ferrites, cobalt spinel ferrites with cubic (FCC) structure possesses potential applications in the fields of high-density data storage [9], catalysis [10], medicine [11], sensors [12] and magnetic recordings [13]. Cobalt ferrites possessing partially inverse spinel structure (i.e. large portion of Co^{2+} occupies the octahedral B sites and the remaining small portion occupies the tetrahedral A sites) exhibits affirmative anisotropy constant [14], huge magnetostriction [15], high electrical resistivity [16] and good chemical stability [17].

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The structural, microstructural, magnetic and electric properties of spinel cobalt ferrite nanoparticles depend upon numerous factors including the way of synthesis, composi- tion of constituents, structure or size and the quantity and type of the substituent [18, 19]. Discrepancy of the cation distribution over A and B sites in the cobalt spinel lattice leads to modified magnetic and electric properties [20]. Many times, the alteration of Fe^{3+}ions with trivalent cations such as Al^{3+}, Nd^{3+}, Gd^{3+}, Ho^{3+}, La^{3+}, and Cr^{3+} in spinel cobalt ferrite is essential to attain definite objectives such as increase of DC resistivity, lowering of saturation mag- netization and the high-temperature applications [21–23]. Spinel cobalt ferrites having two different cation sites offers the prospective for influencing its DC electrical as well as magnetostrictive properties by tailoring the site occupancy preference ability of the cations. This motivated us to carry out the work on trivalent ion-substituted spinel cobalt fer- rite nanoparticles in a systematic manner. The trivalent ions substitution in B site of spinel cobalt ferrite and its effect on the magnetic and electrical properties was studied by many authors [24–28]. But there are only few reports avail- able on structural, morphological, cation distribution and magnetic properties of sol-gel-synthesized Cr^{3+}-substituted spinel cobalt ferrite nanoparticles [29, 30].

Thus, herein, we report sol-gel auto combustion synthesis of trivalent Cr^{3+}-substituted $CoFe_2O_4$ nanoparticles with generic formula $CoCr_xFe_{2-x}O_4$ (where x = 0.0 to 1.0 in the step of 0.2). Further, the effect of trivalent Cr^{3+} ions on
structural, morphological, cation distribution and magnetic properties of $CoFe_2O_4$ nanoparticles were reported.

2 Experimental

2.1 Synthesis Procedure

The A.R. grade citric acid ($C_6H_8O_7.H_2O$), ferric nitrate ($Fe(NO_3)_3.9H_2O$), cobalt nitrate ($Co(NO_3)_2.6H_2O$) and chromium nitrate ($Cr(NO_3)_3.4H_2O$) (>99%) were used as starting materials. The dextrose was used as a fuel. The dextrose to nitrate ratio was considered to be 4:1. The metal nitrates were dissolved together in a minimum amount of deionized water to get a clear solution. An aqueous solution of dextrose was mixed with metal nitrates solution. Then, ammonia solution was slowly added to adjust the pH at
8. The mixed solution was moved on a hot plate with continuous stirring around 80 °C. During evaporation, the solution becomes viscous and finally forms a very viscous brown gel. When finally, all remaining water was released
from the mixture, the sticky mass began to bubble. After several minutes, the gel automatically ignited and burnt with glowing flints. The decomposition reaction would not stop before the whole citrate complex was consumed. The auto ignition was completed within a minute, yielding the brown-coloured ashes termed as per precursor. Further, the samples were fired at 600 °C for 6 h for better crystallinity.

2.2 Characterizations

Roomtemperature x-ray diffraction patterns were recorded using Philips x-ray diffractometer (model 3710, at TIFR Mumbai). XRD patterns were recorded in the 2θ range of 20° to 80° using Cu-Kα radiation. X-ray density (d_x) was evaluated by the mass/volume relation method. The experimental density (d_{exp}) was found using Archimedes's principal, in which the specimen was weighed in air and in xylene at room temperature, ρ_{exp} = weight of the sample in air/loss of weight in xylene. The SEM micrographs of typical samples were recorded using (JEOL-JS-M840 at T.I.F.R. Mumbai) scanning electron microscope. The IR spectra were recorded for all the samples with the help of PerkinElmer spectrometer (Model 783) in the frequency range of 300 to 800 cm^{-1}. The magnetic properties like (M_S), magneton number (nB), and coercively

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(*HC)* are measured using pulse field hysteresis loop technique. The magnetization measurements were carried out in the field of 0.5 Tesla at room temperature.

3 Results and Discussion

3.1 X-ray Diffraction Analysis

The x-ray diffraction patterns of $CoCr_xFe_{2-x}O_4$ (where x= 0.0 to 1.0 in step of 0.2) nanoparticles are shown in Fig. 1a–f. The diffraction patterns and data indicate that all the samples possess cubic spinel structure. The x-ray diffraction pattern shows the reflection namely (220), (311), (222), (422), (400) and (511) which belongs to cubic spinel structure. The Bragg's peaks in the XRD pattern are slightly broader indicating the nano-sized nature of the samples. The most intense peak (311) of the XRD pattern has been considered to determine the particle size of the samples. Scherrer's formula was used to obtain particle size and the values of the particle size for all the compositions are listed in Table 1. It can be seen from Table 1 that the particle size varies from 26 to 38 nm. The XRD data was also used to evaluate cell dimensions (lattice constant *a)*. The values of lattice constant were also given in Table 1.The variation of lattice constant is shown in Fig. 2. It is observed that lattice constant decreases linearly with the substitution of chromium ions and obeys Vegard's law [31]. The decrease in lattice constant in the present study is attributed to the difference in ionic radii of Fe^{3+} and substituent Cr^{3+}. Usually, when ions of larger ionic radii are replaced by the smaller ionic radii in the spinel lattice, the decrease in lattice constant is observed. In the present case Fe^{3+} ions of larger radii (0.67 Å) are replaced by Cr^{3+} ion of smaller ionic radii (0.63 Å) and hence we observed the decrease of the lattice constant with increase in chromium substitution. Similar trend of lattice constant was also reported in chromium substituted cobalt ferrite system [32, 33]. The unit cell volume was also calculated using the values of lattice constant and are listed in Table 1. It is observed that volume of the unit cell decreases with increase in chromium substitution. The x-ray density (d_x) of all the samples was also calculated from XRD data. The values of x-ray density are given in Table 1 and variation is shown in Fig. 3. X-ray density increases with increase in chromium substitution. The x-ray density is in the range of 5.298–5.379 g/cm^3. The bulk density of the specimen has been determined accurately by the hydrostatic method. The values of bulk density are presented in Table 1. The porosity of the samples was calculated using the value of x-ray and bulk densities and are reported in Table 1. The surface area was determined by using the following relation

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Table 1 Values of lattice constant (*a*), crystallite size (*t*), unit cell volume (*V*), x-ray density (*dX*), bulk density (d_B), porosity particles (*P*), grain size (*G*) and specific area (*S*) of $CoCr_xFe_{2x}O_4$ spinel ferrite nanoparticles

Structural parameters	Composition *x*					
	0.0	0.2	0.4	0.6	0.8	1.0
a (Å)	8.379	8.361	8.351	8.331	8.316	8.291
t (nm)	38	35	34	31	27	26
V (Å^3)	588.3	584.5	582.4	578.2	575.1	569.9
d_X (g/cm^3)	5.298	5.315	5.316	5.337	5.348	5.379
d_B (g/cm^3)	4.550	4.610	4.680	4.730	4.760	4.830
P (%)	14.12	13.26	11.96	11.37	10.99	10.21
G (nm)	–	32	–	30	–	–
S (m^2/g)	43.04	39.51	38.37	34.85	30.29	29.00

$S = 6000/\rho d$, where, ρ is x-ray density, d is average particle size and S is surface area. The values of surface area are included in Table 1. It can be observed from Table 1 that all the samples show large surface area and vary with the chromium substitution.

The distance between magnetic ions (hopping length) at tetrahedral A sites and octahedral B sites was calculated for all the samples using the standard relation [34]. The values of hopping length L_A and L_B are given in Table 2. Figure 4 gives the variation of hopping length with the composition *x*. It can be seen from Fig. 4 that both L_A and L_B decreases with chromium content *x*. The observed behaviour of hopping length with chromium content *x* is attributed to decrease in the lattice parameter. The bond length of tetrahedral A site d_{AX} and octahedral B site d_{BX}, tetrahedral edge d_{AXE}, shared octahedral edge d_{BXE} and unshared octahedral edge d_{BXEU} are calculated by using the experimental values of lattice parameter *a* and oxygen positional parameter *u*.The values of allied parameters calculated from above mentioned expression are presented in Table 2. The Table 2 indicates that the tetrahedral bond length d_{AX} and octahedral bond length d_{BX} decreases as Cr^{3+} content *x* increases. Table 2 shows that the tetrahedral edge d_{AXE}, unshared octahedral edge d_{BXEU} does not vary much with Composition while shared octahedral edge d_{BXE} decreases. This could be related to the smaller radius of Cr^{3+} ions as compared to Fe^{3+} ions and the fact that Cr^{3+} occupies strongly tetrahedral B site.

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3.2 SEM Analysis

Scanning electron micrographs (SEM) of the typical samples $x = 0.4$ and $x = 0.6$ is shown in Fig. 5. It can be observed from the SEM images that the prepared samples are amorphous and porous in nature. Particle size obtained by SEM intersect method is of the nanometer dimension and the values are given in Table 1.

Table 2 Values of hopping length of tetrahedral site (LA), octahedral site (LB), ionic radii (rA and rB), oxygen parameter (u), theoretical lattice constant (a_{th}) tetrahedral bond (dAX), octahedral bond (dBX), tetra edge (dAXE), and octa edge (dBXE) of $CoCr_xFe_{2-x}O_4$ spinel ferrite nanoparticles

Structural parameters	Composition x					
	0.0	0.2	0.4	0.6	0.8	1.0
LA (Å)	3.628	3.620	3.616	3.607	3.601	3.590
LB (Å)	2.962	2.956	2.953	2.945	2.940	2.931
rA (Å)	0.683	0.682	0.680	0.679	0.678	0.677
rB (Å)	0.689	0.722	0.756	0.790	0.823	0.857
u (Å)	0.3880	0.3882	0.3883	0.3885	0.3887	0.3891
a_{th} (Å)	8.381	8.368	8.359	8.333	8.320	8.297
dAX (Å)	1.901	1.897	1.895	1.890	1.887	1.881
dBX (Å)	2.048	2.043	2.041	2.036	2.0.32	2.026
dAXE (Å)	3.104	3.097	3.094	3.086	3.081	3.072
dBXE (Å)	2.820	2.814	2.810	2.804	2.799	2.790
	2.970	2.964	2.960	2.953	2.948	2.939

3.3 Cation Distribution

The cation distribution in the spinel ferrite system $CoCr_xFe_{2-x}O_4$ was determined by x-ray intensity ratio calculation method. The details of the method used for the determination of cation distribution were already explained in our previous reports [35]. Similar procedure was adopted in the present study. The results of cation distribution are illustrated in Table 3. It is evident from Table 3 that chromium ions totally occupy octahedral B site, whereas, Co^{2+} and Fe^{3+} ions are partially occupied at tetrahedral

A and octahedral B site. The Fe_A/Fe_B ratio increases with chromium substitution which leads to decrease in magnetization. The variation of iron ratio at B and A sites as a function of composition x is depicted in Fig. 6. Cr^{3+} ions occupy octahedral B site by replacing Fe^{3+} ions. The observed and calculated intensity ratios (Table 3) are in close agreement with each other which suggest that the estimated cation distribution is correct. The mean ionic radius of the tetrahedral A and octahedral B site (rA and rB) can be calculated by the standard relations [36]. The

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values of r_A and r_B are given in Table 3. It is clear that both r_A and r_B decreases with increase in Cr content x. The decrease in r_A and r_B is due to the replacement of Fe^{3+} ions (0.67 Å) by smaller Cr^{3+} ions (0.63 Å) at both sites. The variation of r_A and r_B and oxygen parameter u and variation of ionic radii (r_A and r_B) with x is given in Fig. 6.

The theoretical values of lattice parameter were calcu- lated using the standard equation and the values of theoreti- cal lattice parameter a_{th} are given in Table 3. The theoretical lattice parameter decreases with increase in Cr content x. The variation of theoretical values is similar to that observed for experimentally determined lattice constant.

Infrared Spectroscopy Analysis

Figure 7a–f depicts the IR spectra for $CoCr_xF_{2-x}O_4$ spinel ferrite system under investigation. Two prominent absorption bands are seen in the IR spectra which looks different than the IR spectra of bulk samples. The two major absorption bands are found to be broad, which is attributed to smaller particle dimensions of the samples.

The two absorption bands are assigned to intrinsic vibrations of molecules at tetrahedral A and octahedral B sites and are denoted by υ_1 and υ_2 respectively. The values of υ_1 and υ_2 are given in Table 4. These values are in reported range and are used to determine force constant K_t and K_o [37]. The values of force constant are given in Table 4. It can be seen from the table that K_t and K_o varies significantly with chromium substitution. The values of bond length R_A and R_B obtained from IR data are given in Table 4.

Table 3 Cation distribution, observed and calculated intensity ratios of $CoCr_xFe_{2-x}O_4$ spinel ferrite nanoparticles

Com. x	Cation distribution		$A(Fe)^{3+}/B[Fe]^{3+}$	I (400)/I (440)		I (220)/I (440)	
	A site	B site		Obs.	Cal.	Obs.	Cal.
0.0	$Co_{0.26}Fe_{0.78}$	$Co_{0.74}Fe_{1.26}$	0.587	0.936	1.103	1.360	1.121
0.2	$Co_{0.24}Fe_{0.76}$	$Co_{0.76}Cr_{0.2}Fe_{1.04}$	0.731	0.869	0.611	0.657	0.548
0.4	$Co_{0.20}Fe_{0.80}$	$Co_{0.80}Cr_{0.4}Fe_{0.80}$	1.000	1.111	1.127	1.098	1.002
0.6	$Co_{0.18}Fe_{0.82}$	$Co_{0.82}Cr_{0.6}Fe_{0.58}$	1.414	0.990	0.829	1.000	0.847
0.8	$Co_{0.15}Fe_{0.85}$	$Co_{0.85}Cr_{0.8}Fe_{0.35}$	2.429	1.097	1.044	1.062	1.031
1.0	$Co_{0.14}Fe_{0.86}$	$Co_{0.86}Cr_{1.0}Fe_{0.14}$	6.143	0.947	0.494	1.028	0.499

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3.4 Magnetic Properties

Magnetization measurements for the ferrite system were carried out using the pulse field hysteresis loop technique at 300 K with an applied field of 5 KOe to reach saturation values and the results are plotted as in Fig. 8a–f. Using the
MH plots (Fig. 8a–f) the saturation magnetization (*MS)* was obtained for all the samples.

The variation of saturation magnetization with chromium content is shown in Fig. 9. The saturation magnetization decreases with chromium content. The decrease in magne- tization is associated with the magnetic interaction between A and B sites. In the present ferrite system Fe^{3+} ions of 5 μB magnetic moment are replaced by Cr^{3+} ions of low magnetic moment of 3 μB. This results in decrease in magnetic moment of octahedral B site and hence the net

Table 4 Band positions ($v1$ and $v2$), force constant (K_O and K_t) and bond length (R_A and R_B) of $CoCr_X Fe_{2-x} O_4$ spinel ferrite nanoparticles

Com. x	Band positions		Force constant		Bond length	
	$v1$ (cm^{-1})	$v2$ (cm^{-1})	$K_O \times 10^5$(dyne/cm)	$K_t \times 10^5$(dyne/cm)	R_A	R_B
0.	680	500	1.105	1.760	1.945	0.2440
0.2	660	490	1.116	1.768	1.941	0.2435
0.4	650	448	1.131	1.789	1.938	0.2432
0.6	640	460	1.128	1.775	1.934	0.2426
0.8	635	465	1.179	1.809	1.930	0.2422
1.0	630	469	1.189	1.813	1.924	0.2414

magnetic moment of the system decreases with chromium substitution.

According to Neel's two sub-lattice model of ferri- magnetism, saturation magnetization is given by $M_S = M_B — M_A$ where M_A and M_B are the tetrahedral and octahedral
sub-lattice magnetization [38]. The sub-lattice magnetic moment are calculated using the cation distribution data and taking ionic magnetic moment as 3, 3 and 5 μB for Co^{2+}, Cr^{3+} and Fe^{3+} respectively. The values of Neel's magnetic moment (calculated mag- neton number) are given in Table 5. Figure 10 illustrates the variation of observed and calculated magnetic moment as a function of chromium composition x. It is evident from Fig. 10 that both observed and calculated magneton number (n_B) decreases linearly with chromium substitution. The observed and calculated magneton number differs from each other. The remanence magnetization (M_r) and coercivity (H_C) obtained from *MH* plots decreases with chromium composition x. The values of M_r and H_C are given in Table 5. The large values of coercivity as can be seen from Table 5 are due to the smaller particle size of the samples. Due to the substitution of chromium ions these magnetic

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Table 5 Magnetization parameters and magneton number (n_B) of $CoCr_xFe_{2-x}O_4$ spinel ferrite nanoparticles number n_B (μ_B)

	Magnetization parameters				Magneton	
Com. *x*	*Mr* (emu/g)	*MS* (emu/g)	*Mr* /*MS*	*HC* (Oe)	Obs.	Cal.
0.	43.62	67.93	0.64	2329	2.85	3.56
0.2	33.86	57.01	0.59	1480	2.39	3.04
0.4	16.88	41.64	0.41	429	1.74	2.40
0.6	11.5	28.83	0.40	374	1.20	1.88
0.8	4.86	19.46	0.25	197	0.81	1.30
1.0	1.87	5.93	0.32	151	0.25	0.84

Conclusion

The following conclusions were drawn from the present study:

- The samples of $CoCr_xFe_{2-x}O_4$ were successfully synthesized by sol-gel auto combustion method.
- Using sol-gel method, the particle size of about 26–38 nm was achieved.
- The lattice parameter decreases with chromium substi- tution.
- Cation distribution studies revealed that Co^{2+} and Fe^{3+} occupy both A and B sites, whereas Cr^{3+} ions occupy only B site.
- Large values of surface area were observed for present samples.
- Microstructure studied by SEM technique, shows nanosized nature of the samples.
- The broad absorption bands were seen in IR spectra.
- Saturation magnetization, remanence magnetization and coercivity decreases with increase in chromium substitution.
- Observed and calculated magneton number both decreases with chromium substitution.

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Schiff Bases of Acenaphthoquinone: An Important Bioactive Compound

Kuldeep B. Sakhare[1], Hansaraj Joshi[2*]
[1]Department of Chemistry, Balbhim Arts, Science & Commerce College, Beed-431122, Maharashtra,
[2]Department of Chemistry, Swa. Savarkar Arts, Commerce & Science College Beed, Maharashtra-431122, Maharashtra, INDIA
E-mail: hansarajjoshi307@gmail.com

Abstract: Recently more and more focus is given on the synthesis of novel chemical drugs effective to the various diseases such as cancer, diabetics, fungal, bacterial, Alzheimer etc. as the peoples are facing the problem of these diseases throughout the world. Diagnosis of these diseases and making effective drugs against these diseases is became a challenge to the researcher as well as scientists. In this review article we have presented the method of synthesis and applications of the Schiff base ligand synthesized by condensation of acenaphthoquinone and various primary amine.

Keywords: Metal Complex, Anticancer, Novel, Grinding, Condensation.

1. Introduction:

The term Schiff base was firstly put by the Germen scientist Hugo Schiff in 1864, for this work he has been awarded by Nobel Prize. As the Schiff base include the condensation between aromatic aldehyde and primary amine; it enhances the applications in various fields like medicinal, industrial, agriculture, drug discovery etc. The world's largest population is facing the problem of various diseases, in these the top most diseases are mainly Cancer, Alzheimer, Diabetics etc. It has become challenge for the scientist to control these diseases or to reduce the strength of these diseases. For this reason scientist as well as researcher are very busy in finding novel and effective drugs against these diseases. In the last three decades the coordination chemistry specially complexes of Schiff base ligand is focused very strongly because of its broad spectrum regarding the various biological activities. Antibacterial, antifungal, antiviral, ant malarial, antitumor, ant tuberculosis, anthelmintic, anti-HIV, antidiuretic, anti-inflammatory, antiviral, antiprotozoal, anticonvulsant, analgesic, antioxidant, anti-Alzheimer, anti-hypertension, anti-ulcer, herbicidal properties of Schiff base metal complexes have made them important and have attracted the attention of scientists and researchres. [1-13].

In addition to the Schiff base ligand if metal salts are coordinated then it enhances all the activities in the various fields such as antibacterial, antifungal, anticancer[14]. Due to this there is a continuing interest in developing metal complexes of Schiff bases due to the presence of both hard nitrogen or oxygen and soft sulphur donor atoms in the backbones of these ligands. They readily coordinate with a wide range of transition metal ions yielding stable and intensely coloured metal complexes, some of which have been shown interesting physical and chemical properties and potentially useful biological activities. Acenaphthoquinone is one of the most useful moieties in the development of coordination compounds especially in the transition metal salts. Acenaphthoquinone has two carbonyl groups present in adjacent to each other allowing various amines to bind independently[15].

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2. Experimental:

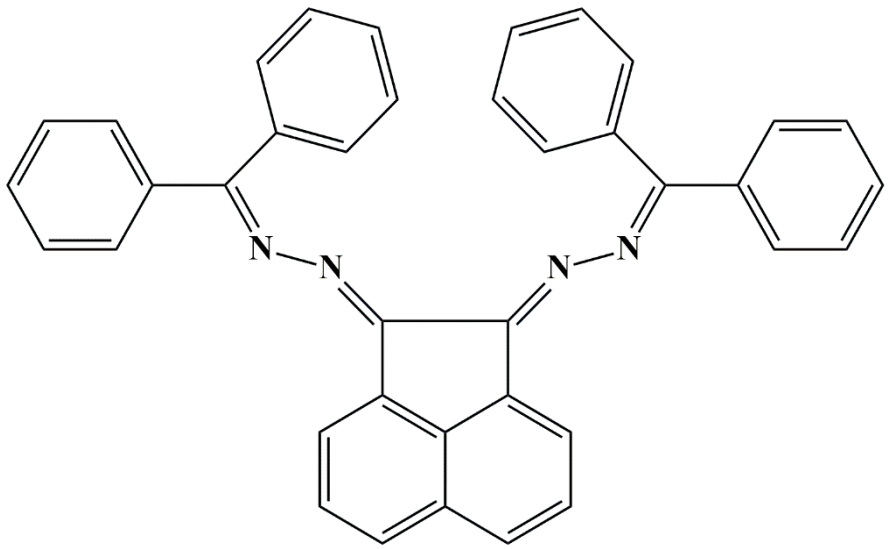
2.1 Materials and Methods:

Synthesis of Schiff base ligand with the help of acenaphthoquinone is quiet easy due to its availability in easy way, cheap purchasing rates and high reactivity with primary amines.

There are plenty of methods to prepare Schiff base ligands by condensing the acenaphthoquinone with amines. One can utilise the common traditional method to prepare Schiff base ligand as many researchers does. Alternatively researchers may adopt green approach and avoid traditional method for this purpose. In this article, following different methods have been explained to prepare Schiff base ligands by acenaphthoquinone.

Chao-Zhi Zhang et al.[16]: have prepared new Schiff base, acenaphthoquinone bis(diphenylmethlenehydrazone) by simple condensation reaction of acenaphthoquinone and diphenylmethylenehydrazone in the combination ratio of 1:2 mole. In addition to this they have coordinated this Schiff base ligand to the metal salts of Silver and Copper as shown in scheme 1 and Scheme 2.

Scheme 1.



Scheme 1. Schiff base ligand prepared by Acenaphthoquinone.

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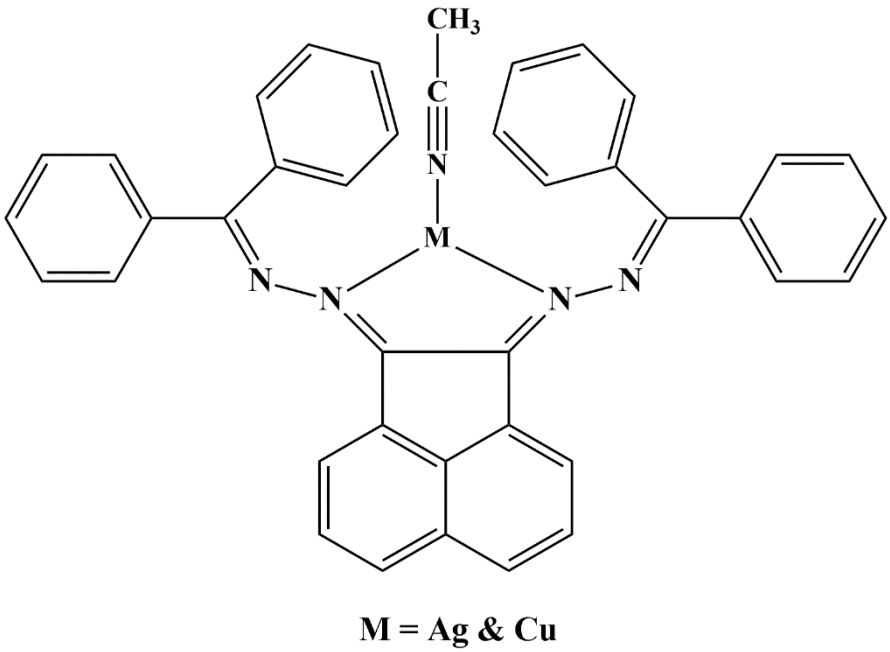
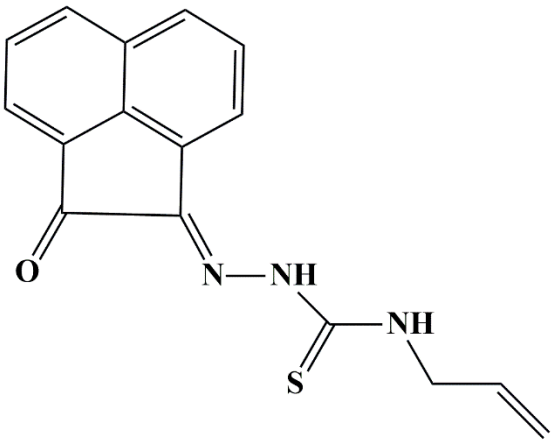
Scheme 2.



Scheme 2. Metal Complexes Prepared by Acenaphthoquinone.

Khlood s. et al. [17] prepared Schiff base ligand along with metal complexes with the help of N(4)-allyl-thiosemicarbazide condensing with Acenaphthoquinone. For the complexation of this Schiff base ligand they utilized the Cobalt, Nickel and Zinc metal salts. Shown in Scheme 3 and 4.

Scheme 3. Preparation of Schiff base ligand from N(4)-allyl-thiosemicarbazide and Acenaphthoquinone.



Scheme 3. Preparation of Schiff base ligand from N(4)-allyl-thiosemicarbazide and Acenaphthoquinone

Scheme 4. Metal Complex of Acenaphthoquinone:

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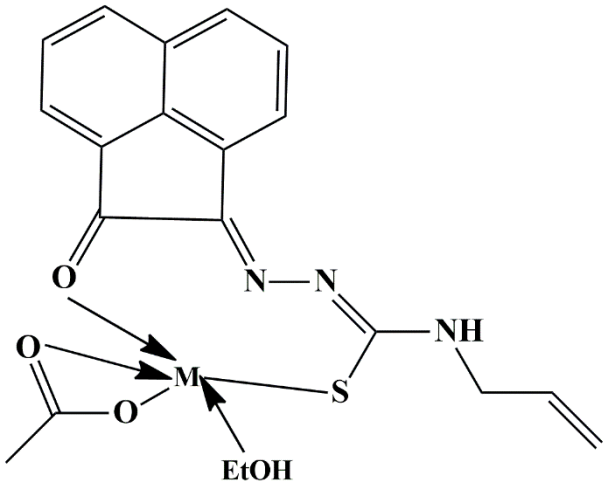
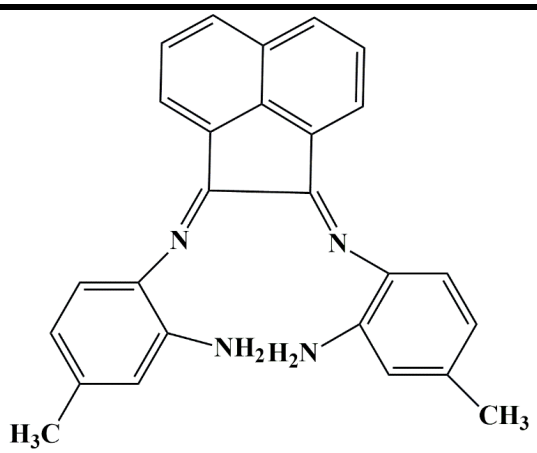


M = Co, Ni and Zn

Scheme 4. Metal Complex of Acenaphthoquinone.

Qusay H.Al-Hialy and Khansaa Sh. Al-Nama[18] prepared simple Schiff base ligand and metal complexes of acenaphthoquinone with condensation of 4-methyl-o-phenylenediamine shown in scheme 5 and 6.

Scheme 5. Preparation of Schiff base ligand from acenaphthoquinone and 4-methyl-o-phenylenediamine:



Scheme 5. Preparation of Schiff base ligand from acenaphthoquinone and 4-methyl-o-phenylenediamine

Scheme 6. Metal Complexes of Acenaphthoquinone:

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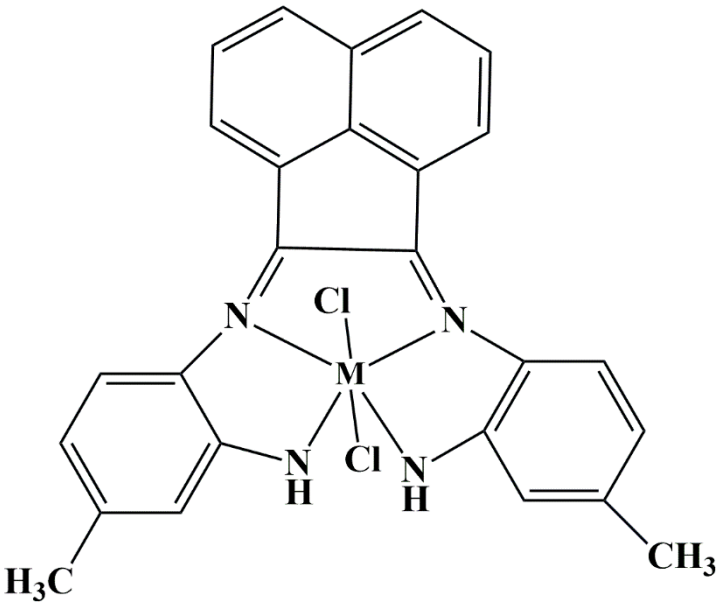
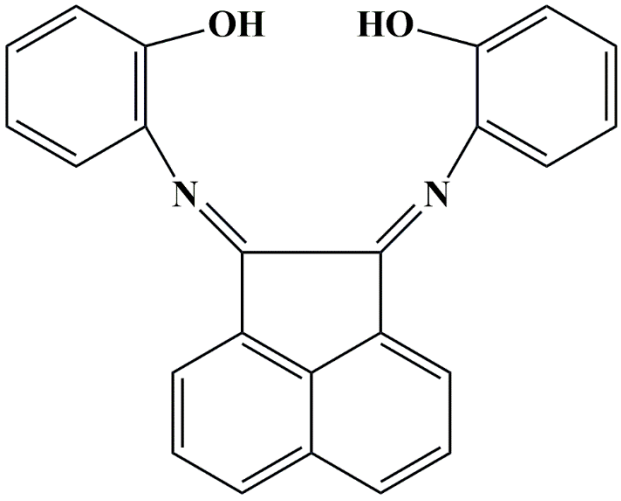


Scheme 6. Metal Complexes of Acenaphthoquinone.

Arumugam et al.[19] have reported synthesis of Schiff base ligand and its metal complexes of Co(II), Ni(II), Cu(II) and Zn(II) shown in scheme 7 and 7 respectively.

Scheme 7: Synthesis of Schiff base ligand of acenaphthoquinone:



Scheme 7: Synthesis of Schiff base ligand of acenaphthoquinone.

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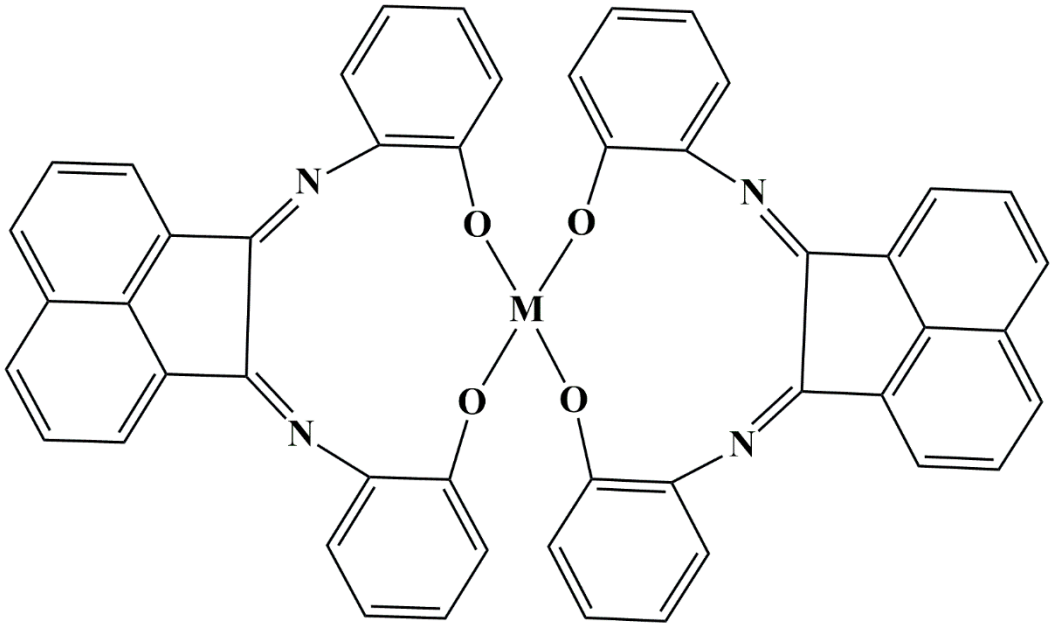
Scheme 8: Synthesis of Metal Complexes:



Scheme 8: Synthesis of Metal Complexes.

3. Result and Discussion:

As discussed above all scheme represents the synthesis of Schiff base ligands and coordination of metal salts to the Schiff base ligand for developing metal complexes. Each scheme was analysed by various spectroscopic techniques such as FTIR, ^{1}H-NMR, Mass, Powder XRD, Thermo gravimetric analysis etc. to confirm that whether the synthesis of Schiff base ligand and metal complexes has been taken place or not. Further these all compounds were scanned by various biological activities to check biological potential of these compounds.

3.1 Applications of Schiff base ligand of Acenaphthoquinone:

3.1.1 Antimicrobial:

The Schiff base ligand has played vital role in various biological activities among these antibacterial and antifungal activities are also included. The Schiff base ligands made by condensation of acenaphthoquinone shows broad peak of activity. In addition to it, if metal salts are coordinated then the spectrum of activity get enhance [20]. The Schiff base ligand synthesized by the acenaphthoquinone and N(4)-allyl-thiosemicarbazideshown have shown good activities. These activities have found enhanced after coordination with metal salts [18]. The Schiff base ligand prepared by the acenaphthoquinone and 1,8-diaminonaphthalene to make macromolecule shows the good antimicrobial activities and it increases after the formation of metal complexes [21].

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3.1.2 Antioxidant Activity:

Antioxidant activity refers to the ability of a substance to neutralize or scavenge free radicals and reactive oxygen species (ROS), which are harmful by-products of cellular metabolism that can damage cells and tissues. Free radicals can contribute to the aging process and are linked to various diseases, such as cancer, cardiovascular diseases and neurodegenerative disorders. Antioxidants play a key role in protecting the body from oxidative stress and maintaining health. The antioxidant activity of Schiff base ligand prepared by acenaphthoquinone has played vital role in the activity of antioxidant [17].

4. Conclusion:

Schiff base ligand synthesized by the condensation of acenaphthoquinone and various primary amines are active in all relevant fields especially in biological activities. The methods of preparation of Schiff base ligand of acenaphthoquinone is very simple as compared to other reactions. After developing metal complexes of these Schiff base ligand, all activities such as antibacterial, antifungal, antiviral, antioxidant, antitumor etc. get enhanced. After the broad literature survey it is clear that there is large scope in the area of the research related to the acenaphthoquinone.

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Synthesis and Antimicrobial Activity Evaluation of-2, 4-(Substituted-Phenyl)-2, 3-Dihydro-1*H*-1, 5-Denzodiazepine Derivatives

Kendre Madhav Marotirao
Department of Chemistry, Shri Sant Gadge Maharaj Mahavidyalaya Loha, Dist. Nanded - 431708, Maharashtra, India

Abstract:

A series of-2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine derivatives (**2a-j**) have been synthesized by the treatment of 1-(substituted-2-hydroxy-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (**1a-j**) with 4-methyl-ortho-phenylene diamine and few drops of piperidine using 20 ml methanol as a solvent was refluxed for 4 hrs. Then glacial acetic acid (5 ml) was added to the reaction mixture and refluxing was continued for 2 hrs, after completion of reaction (checked by TLC). The reaction mixture was left overnight at room temperature. In 70-80% yield with high purity, characterization of compounds was confirmed by the IR, ^{1}H NMR and mass spectral analysis. All these newly synthesized compounds were evaluated for their antibacterial activity against four different pathogens such as *Escherichia coli, Salmonella typhi, Staphylococcus aureus* and *Bacillus subtilis* and antifungal activity against *Aspergillus niger, Penicillium chrysogenum, Fusarium moneliforme* and *Aspergillus flavus,* using Penicillin and Greseofulvin using Peniciline and Greseofulvin as standard drugs by agar cup method and Poison plate method, respectively.

Keywords: 2-Hydroxy-chalcones, ortho-phenylene diamine, 1, 5-Benzodiazepines, Antimicrobial activity.

Corspondance to author
Dr. Kendre Madhav Marotirao
Assistant Professor, Department of Chemistry,
Shri Sant Gadge Maharaj Mahavidyalaya, Loha, Nanded,(M.S.) India-431708.
E-mail:- madhavkendre72@gmail.com
Mobile No.996090778

1. Introduction

In recent time millions of heterocyclic compounds were synthesized due to their specific activity are employed in the treatment of many infectious diseases. Their use in the treatment is attributed to their inherent toxicity of various pathogens. Among a wide range of heterocyclic compounds that have been explored for the development of pharmaceutically important molecules [1-2]. Most of the heterocyclic compounds are well known due to their biological importance. Out of these 1, 5-benzodiazepines are important seven member heterocyclic molecules which represent a variety of biological activities [3-4] and various methods have been worked out for the synthesis of 1, 5-benzodiazepine derivatives. Several 1, 5-benzodiazepine compounds possess important pharmacological activities [5] Most of the 1, 5-benzodiazepine derivatives display a broad spectrum of pharmacological activities such

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as antibacterial[6-7], antifungal[8], antitubercular[9-10], cytotoxic[11], anti-inflammatory[12], antioxidant[13-14], anticancer[15], anticonvulsant[16-17], Antidepressant[18-19], Sedative [20], agents. 1, 5-benzodiazepine derivatives have been found to possess considerable biological activities [21-22]. The literature survey shows interesting biological activities [23-24] and the development of 1, 5-benzodiazepine as a potential antimicrobial agent. Therefore; our interest to synthesize some novel 1, 5-benzodiazepine molecules and evaluated them as promising antimicrobial agents. In view of these observations, in the present investigation we report herein, 2-hydroxy-chalcone condensed with substituted-ortho-phenylene diamine to obtain the final 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-Benzodiazepine derivatives **(2a-j),** having halogen and dimethylamino groups as increasing antimicrobial activities.

2. Materials and Methods

All the solvents and reagents were obtained from commercial sources and were used without further purification. The melting points were determined by Open Capillary method and are uncorrected. The mass spectra were obtained with a Shimadzu GC-MS spectrophotometer. The IR spectra in KBr were recorded on Shimadzu Spectrophotometer and ^{1}H NMR spectra were recorded in DMSO on Avance 300 MHz Spectrometer using TMS as internal standard. The chemical shift values are expressed in part per million (ppm) downfield from the internal standard and signals are quoted as s (singlet), d (doublet), t (triplet) and m (multiplet). Thin-layer chromatography (TLC) was used to monitor the progress of all reactions and to check the purity of compounds by using ethyl acetate and petroleum ether as an eluent in the ratio of (3:7 v/v). All the newly synthesized 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-Benzodiazepine (**2a-j**) compounds were tested for their antimicrobial activities by agar cup method and Poison plate method, respectively.

General method for the Synthesis of 2**, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-Benzodiazepine derivatives**

An equimolar reaction mixture of (0.001 mol) 1-(substituted-2-hydroxy-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one and 4-methyl-ortho-phenylene diamine (0.001 mol) in presence of few drops of piperidine using 20 ml of methanol as a solvent was refluxed for 4 hrs. Then glacial acetic acid (5 ml) was added to the reaction mixture and refluxing was continued for 2 hrs. The progress of the reaction was monitored by using TLC [eluent: ethyl acetate; petroleum ether (3:7)], after completion of reaction (checked by TLC). The reaction mixture was left overnight at room temperature. The reaction mixture was poured on crushed ice-cold water. The solid crude product obtained was filtered, washed with cold water, dried and recrystallized by using ethanol to get corresponding 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-Benzodiazepine compounds in 70-80 % yield.

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Scheme-1: Synthesis of 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-Benzodiazepine derivatives

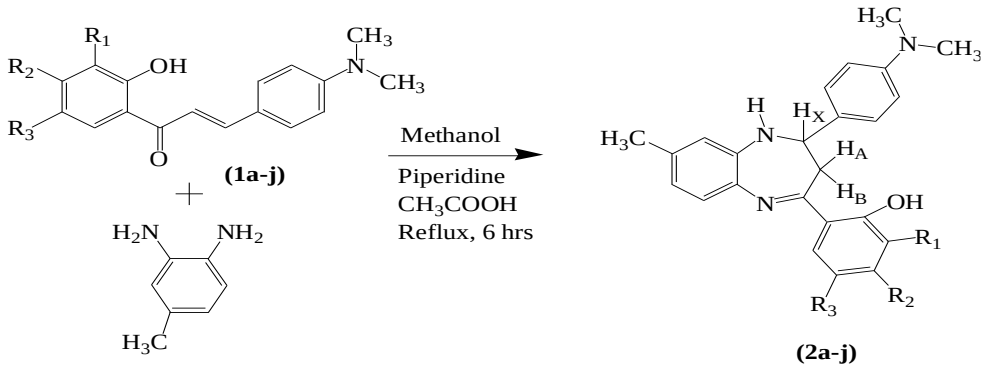

Table-1: Physical data of synthesized 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine derivatives (2a-j)

Sr. No.	Entry	R_1	R_2	R_3	Molecular Formula	Molecular weight	Yield in (%)	Melting Point ^{0}C
1	**2a**	I	H	I	$C_{24}H_{23}N_3I_2O$	623	75	137-138
2	**2b**	I	H	CH_3	$C_{25}H_{26}N_3IO$	511	75	134-135
3	**2c**	Cl	H	Cl	$C_{24}H_{23}N3Cl_2O$	441	80	126-127
4	**2d**	I	H	Cl	$C_{24}H_{23}N_3IClO$	531	75	122-123
5	**2e**	Br	H	CH_3	$C_{25}H_{26}N_3BrO$	464	70	144-145
6	**2f**	Br	H	Cl	$C_{24}H_{23}N_3BrClO$	484	78	147-149
7	**2g**	Br	H	Br	$C_{24}H_{23}N_3Br_2O$	529	78	157-158
8	**2h**	I	H	Br	$C_{24}H_{23}N_3IBrO$	576	76	143-144
9	**2i**	H	CH_3	Cl	$C_{25}H_{26}N_3ClO$	419	75	135-136
10	**2j**	H	H	Br	$C_{24}H_{24}N_3BrO$	450	80	124-126

3. Antimicrobial Activity

3.1. Antibacterial activity

All the synthesized 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-Benzodiazepine compounds (**2a-j**) were assessed for their antibacterial and antifungal activities against four different strains of bacteria such as *E. coli*, *S typhi*, *S. aureus* and *B. subtilis* and four fungi like *Aspergillus niger*, *Penicillium chrysogenum*, *Fusarium moneliforme and Aspergillus flavus*. The test for antibacterial activity was carried by agar cup method [25-26] (cup size 8 mm) with nutrient agar as medium whereas antifungal activity was carried out by using potato-dextrose agar (PDA) medium by same agar cup plate method. All synthesized compounds were dissolved in DMSO and used as control concentration of each test

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compound was 100µg/ml. The experiments were performed in triplicate in order to minimize the errors. Zone of inhibition were recorded after incubation at 37 ^{0}C for 24 hrs, zone of inhibition produced by each compound was measured in mm. After incubation plates were observed for the zone of inhibition of bacterial growth around the agar cup. Results were recorded by measuring the zone of inhibition in millimeter (mm) using zone reader. All the newly synthesized 1, 5-benzodiazepine compounds were evaluated for their antibacterial activity against the selected four different pathogens, such as E. coli, S. typhi, *S. aureus* and *B. subtilis*. The **2e,** of substituted 1, 5-benzodizepine compounds show maximum activity against E. coli while compounds **2f** and **2j** show weak activity against E. *coli*. The synthesized compounds of benzodiazepine **2b** and **2f** showed maximum activity against *S.* typhy and compound **2c** and **2g** shows moderate activity as compare to standard drug. The compounds **2a**, **2c** and **2i** showed significant activity against *S. aureus* as compared with standard drugs.

Table No. 2: Antibacterial activity data of 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine derivatives (2a-j)

Sr. No.	Entry	molecular formula	Antibacterial activity (Zone of Inhibition in mm)			
			Escherichia coli	*Salmonella typhi*	*Staphylococcus aureus*	*Bacillus subtilis*
1	**2a**	$C_{24}H_{23}N_3I_2O$	12	17	21	14
2	**2b**	$C_{25}H_{26}N_3IO$	14	18	--	12
3	**2c**	$C_{24}H_{23}N_3Cl_2O$	12	14	22	11
4	**2d**	$C_{24}H_{23}N_3IClO$	14	--	17	14
5	**2e**	$C_{25}H_{26}N_3BrO$	15	11	--	15
6	**2f**	$C_{24}H_{23}N_3BrClO$	11	18	18	16
7	**2g**	$C_{24}H_{23}N_3Br_2O$	13	16	17	13
8	**2h**	$C_{24}H_{23}N_3IBrO$	12	--	18	16
9	**2i**	$C_{25}H_{26}N_3ClO$	14	--	22	18
10	**2j**	$C_{24}H_{24}N_3BrO$	11	16	16	12
+ve Control DMSO			**-ve**	**-ve**	**-ve**	**-ve**
Penicilline			**12**	**20**	**34**	**22**

(-- = No Antibacterial activity

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3.2. Antifungal activity

The antifungal activity of substituted 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine derivatives (**2a-j)** were screened against four plant pathogenic and mold fungi, such as *Aspergillus niger, penicillium chrysogenum, Fusarium moneliforme and Aspergillus flavus.* The antifungal activities of the synthesized 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine derivatives (**2-j)** were assessed by poisoned plate method [27-28]. Griseofulvin (100µg/disc) was used as standard drug for the antifungal test. Potato Dextrose Agar (PDA) was used as basal medium for test fungi. The compound 100 µg were mixed with sterilized potato dextrose agar (PDA) medium at 40 ^{0}C of the rate 100 mg/mL PDA. The medium was poured in sterilized Petri-plates and allowed solidified PDA media and then incubated at 30 ^{0}C for 72 hours. The growth of fungal area was measured in mm after 4 days of incubation at 30 ^{0}C. A control set was maintained using only PDA with DMSO as growth medium. Results were measured as the growth of fungi (does not show antifungal activity), reduced growth of fungi (to observed moderate antifungal activity), and no growth of fungi (antifungal activity observed in the area). All synthesized compounds were evaluated for their antifungal activity against the four different pathogens *Aspergillus niger*, *Penicillium chrysogenum*, *Fusarium moneliforme* and *Aspergillus flavus*. The antifungal activity of some 1, 5-benzodiazepine compounds showed good activity against four pathogens. The presence of halogen and –N(CH_3)$_2$ groups were found to responsible for increasing antimicrobial activity.

Table No. 3: Antifungal activity data of 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine derivatives (2a-j)

Sr. No.	Entry	molecular formula	Antifungal activity (Zone of Inhibition in mm)			
			Aspergillus niger	*penicillium chrysogenum*	*Fusarium moneliforme*	*Aspergillus flavus*
1	**2a**	$C_{24}H_{23}N_3I_2O$	RG	-ve	RG	-ve
2	**2b**	$C_{25}H_{26}N_3IO$	-ve	-ve	-ve	RG
3	**2c**	$C_{24}H_{23}N_3Cl_2O$	RG	-ve	RG	RG
4	**2d**	$C_{24}H_{23}N_3IClO$	-ve	RG	RG	RG
5	**2e**	$C_{25}H_{26}N_3BrO$	RG	RG	-ve	-ve
6	**2f**	$C_{24}H_{23}N_3BrClO$	-ve	RG	RG	-ve
7	**2g**	$C_{24}H_{23}N_3Br_2O$	-ve	RG	-ve	RG
8	**2h**	$C_{24}H_{23}N_3IBrO$	RG	-ve	-ve	RG
9	**2i**	$C_{25}H_{26}N_3ClO$	-ve	-ve	RG	-ve
10	**2j**	$C_{24}H_{24}N_3BrO$	RG	RG	-ve	-ve

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+ve Control DMSO	**+ve**	**+ve**	**+ve**	**+ve**
-ve Control (Griseofulvin)	**-ve**	**-ve**	**-ve**	**-ve**

[+ve = No growth (Antifungal activity absent), RG = Reduced Growth (more than 50 % but less than 90 % i. e.Moderate Activity), -ve = No Growth (Antifungal Activity Observed 90 %)]

4. Results and Discussion

In the present work a series of some novel 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine derivatives (**2a-j**) were synthesized by cyclization of corresponding 3-(4'-dimethylamino-phenyl)-1-(substituted-2-hydroxy-phenyl)-propenone (2-hydroxychalcone) derivatives (**1a-j**) and substituted ortho-phenylene diamine. The uses of different chalcone for the synthesis of 1, 5-benzodiazepine derivatives have been investigated. The presence of halogen and dimethylamino group in different position of benzene ring of the chalcone and the use of substituted ortho-phenylene diamine resulted in synthesis of 1, 5-benzodiazepine derivatives with significantly high yield. All these products of 1, 5-benzodiazepine derivatives didn't give pink coloration with concentrated H_2SO_4 solution. The structures of newly synthesized compounds have been confirmed by IR, ^{1}H NMR and Mass spectral data. The IR spectrum of compound **2i** exhibited peaks due to group -C=N, at 1572 cm-^{1}. The ^{1}H NMR spectrum shows characteristic peaks dd at δ 2.0-2.1 of H_A and δ 2.3-2.4 of H_B respectively due to proton of methylene group of seven member diazepine ring, due to germinal and vicinal coupling of -CH_2 protons of the diazepine ring. Further, the -CH proton of the ring resonated as a triplet at δ 4.2-4.4 (t, 1H, H_X), due two vicinal coupling with the two non-equivalent protons of the methylene group at position three of the diazepine ring. The proton of >N-H singlet shows at pick δ 4.5-4.8 (s, 1H, >NH), and the pick of CH_3 group in ortho-phenylene dianime shows at δ 2.1-2.2 (s, 3H, CH_3) and dimethylaminine shows at δ 2.85-3.0 (s, 6H, -N(CH_3) also sharp pick of -OH group at δ 11.0-11.3 (s, 1H, OH), these observations are in agreement with the spectral data reported by different researcher [29-31]

All the newly synthesized 1, 5-benzodiazepine compounds were evaluated for their antibacterial activity against the selected four different pathogens, such as E. coli, S. typhi, *S. aureus* and *B. subtilis*. The **2e,** of substituted 1, 5-benzodizepine compounds show maximum activity against E. coli while compounds **2f** and **2j** show weak activity against E. *coli*. All the synthesized compounds of benzodiazepine **2b** and **2f** showed maximum activity against *S.* tiphy and compounds **2c** and **2g** shows moderate activity as compare to standard drug. The compounds **2a**, **2c** and **2i** showed significant activity against *S. aureus* as compared with standard drugs. All the newly synthesized compounds were evaluated for their antifungal activity against the four different pathogens *Aspergillus niger*, *Penicillium chrysogenum*, *Fusarium moneliforme* and *Aspergillus flavus*. The antifungal activity of some 1, 5-benzodiazepine compounds showed good activity against four pathogens. The presence of halogen and –N<(CH_3)$_2$ groups were found responsible for increasing antimicrobial activity.

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Spectroscopic data of synthesized compounds

4-(3, 5-dichloro-2-hydroxy-phenyl)-2-(4'-dimethylamino-phenyl)-8-methyl-2, 3-dihydro-1*H*-1, 5-benzodiazepine (2c):- **IR (KBr):-** 3368 (>N-H), 3286 (Ar-OH), 1568 (>C=N), 1464 (>C=C<), 724 (>C-Cl) cm^{-1}; **^{1}H NMR(DMSO):-** δ 2.1-2.3 (s, 3H, CH_3) δ 2.85-3.0 (s, 6H, -$N(CH_3)_2$), δ 2.0-2.1 (dd, 1H, H_A), δ 2.3-2.4 (dd, 1H, H_B), δ 4.1-4.4 (t, 1H, H_X), δ 4.5-5.0 (s, 1H, >NH), δ 6.7-7.7 (m, 9H, Ar-H), δ 11.0-11.3 (s, 1H, OH, D_2O exchangeable); **MS** (m/z); 441 (M+1)

4-(3-Bromo-5-methyl-2-hydroxy-phenyl)-2-(4'-dimethylamino-phenyl)-8-methyl-2, 3-dihydro-1*H*-1, 5-benzodiazepine (2e):- IR (KBr):- 3358 (>N-H), 3284 (Ar-OH), 1573 (C=N), 1468 (>C=C<), 735 (C-Br), cm-^{1}; **^{1}H NMR(DMSO)**:- δ 2.1-2.3 (s, 6H, CH_3), δ 2.85-3.0 (s, 6H, -$N(CH_3)_2$), δ 2.0-2.1 (dd, 1H, H_A), δ 2.1-2.3 (dd, 1H, H_B), δ 4.1-4.4 (t, 1H, H_X), δ 4.5-4.9 (s, 1H, >NH), δ 6.5-7.5 (m, 9H, Ar-H), δ 11.0-11.2 (s, 1H, OH, D_2O exchangeable); **MS** (m/z):- 464 (M+1)

4-(5-Chloro-4-methyl-2-hydroxy-phenyl)-2-(4'-dimethylamino-phenyl)-8-methyl-2,3-dihydro-1*H*-1, 5-benzodiazepine (**2i**):- IR (KBr):- 3366 (>N-H), 3278 (Ar-OH), 1572 (C=N), 1462 (>C=C<), 725 (C-Cl), cm-^{1}; **^{1}H NMR(DMSO)**:- δ 2.1-2.3 (s, 6H, CH_3), δ 2.85-3.0 (s, 6H, -$N(CH_3)_2$), δ 2.0-2.2 (dd, 1H, H_A), δ 2.0-2.3 (dd, 1H, H_B), δ 4.2-4.4 (t, 1H, H_X), δ 4.5-4.8 (s, 1H, >NH), δ 6.7-7.7 (m, 9H, Ar-H), δ 11.2-11.3 (s, 1H, OH, D_2O exchangeable); **MS** (m/z):- 419 (M+1)

4-(4-Bromo-2-hydroxy-phenyl)-2-(4'-dimethylamino-phenyl)-8-methyl-2,3-dihydro-1*H*-1, 5-benzodiazepine (**2j**):- IR (KBr):- 3372 (>N-H), 3268 (Ar-OH), 1565 (C=N), 1467 (>C=C<), 735 (C-Br), cm-^{1}; **^{1}H NMR(DMSO)**:- δ 2.1-2.3 (s, 3H, CH_3), δ 2.85-3.0 (s, 6H, -$N(CH_3)_2$), δ 2.0-2.2 (dd, 1H, H_A), δ 2.0-2.2 (dd, 1H, H_B), δ 4.2-4.5 (t, 1H, H_X), δ 4.5-4.8 (s, 1H, >NH), δ 6.6-7.5 (m, 10H, Ar-H), δ 11.0-11.3 (s, 1H, OH, D_2O exchangeable); **MS** (m/z):- 450 (M+1)

Conclusion

In this work, we have demonstrated the synthesis of 2, 4-(substituted-phenyl)-2, 3-dihydro-1*H*-1, 5-benzodiazepine (**2a-j**) compounds using simple experimental procedure with high yield, relatively short reaction time and low cost. All the synthesized compounds were screened for their antibacterial and antifungal activities. From the result of antibacterial **2e,** of substituted 1, 5-benzodizepine compounds show maximum activity against E. *coli* while compounds **2f** and **2j** show weak activity against E. *coli*. The compounds **2a**, **2c** and **2i** showed significant activity against *S. aureus* as compared with standard drug. The antifungal activity of some benzodiazepine compounds showed good activity against four selected pathogens. The presence of halogen and –$N<(CH_3)_2$ groups were found responsible for increasing antimicrobial activity.

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Conflict of Interest

The authors declare no conflict of interest.

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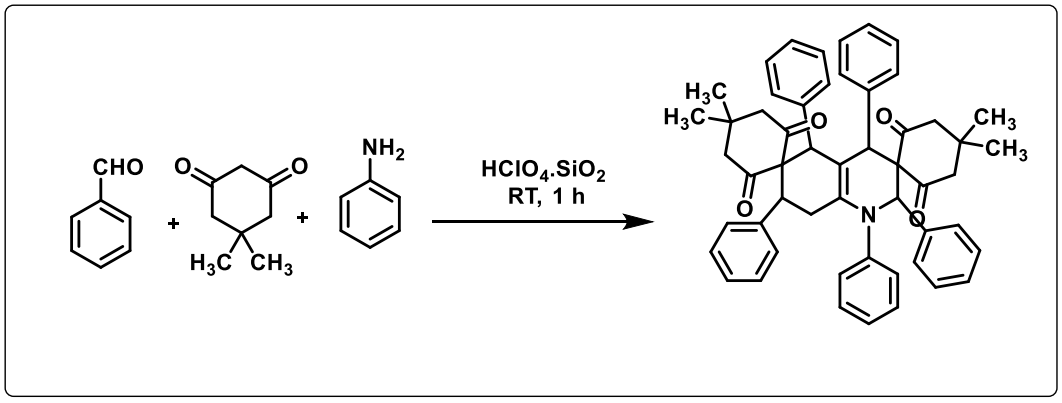
Benign Chemistry of dispiro-hydroquinolines via a one-pot Multicomponent reaction

Pawde Shubhangi S., D. B.Muley
Research Centre & PG Department of Chemistry, Shivaji Mahavidyalaya, Udgir 413517
Email: muleydb@gmail.com

Abstract

A protocol has been developed for the synthesis of dispiro [tetrahydroquinoline-bis(5,5-dimethylcyclohexane-1,3-dione] derivatives via a one-pot multicomponent reaction of aryl amines, aromatic aldehydes, and Dimidone . Silica supported perchloric acid ($HClO_4$-SiO_2) was used as an efficient catalyst for the synthesis of dispiro[tetrahydroquinoline-bis(5,5-dimethylcyclohexane-1,3-dione] derivatives. The products were successfully synthesized in solvent free conditions and room temperature along with the suggested mechanism through combination of domino Knoevenagel, Michael, and Diels–Alder reactions. The remarkable advantages offered by this method are inexpensive catalyst, good yields, simple and easy work-up procedure. The products have been characterized by IR, mass, 1H NMR, ^{13}C NMR spectroscopy, and elemental analysis. The compounds synthesized were examined through biological activities.

Keywords: Aromatic aldehydes, Aromatic amines, Dimidone, Dispiro compounds



1.Introduction

Multicomponent reactions allow the creation of several bonds in a single operation and are attracting increasing attention as one of the most powerful emerging synthetic tools .Multicomponent reactions are defined as domino reactions involving at least three substrates. The use of multicomponent reactions in organic synthesis is increasing constantly. Such single-step reactions allow the synthesis of a wide range of complex molecules, including natural products and biologically active compounds such as pharmaceuticals and agrochemicals, in an economically favourable way by using processes that are reasonably simple. In domino reactions, two or more bond-forming transformations occur on the basis of functionalities formed in the previous step. Furthermore, no additional reagents, catalysts, or additives can be added to the reaction vessel nor can reaction conditions be changed. These reactions allow the efficient synthesis of complex molecules from simple substrates in an ecologically and economically favourable way.

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Hydroquinoline ring system is an important structural unit in a many naturally occurring alkaloids and therapeutics. Hydroquinolines have attracted great interest from synthetic, biogenic, and biological points of view. They exhibit significant pharmacological activities, dopamine D2-receptor, agonist to serotonin, and inhibitory activity against acetylcholinesterase, and they were used in treatment of disorders Also, spirocyclic compounds including a dimidone unit are attractive intermediates in the synthesis of natural products and in medicinal chemistry and are also the starting materials for the synthesis of exotic amino acids that are used to modify the physical properties and biological activities of peptides, peptidomimetics, and proteins . Thus, the synthesis of a new highly substituted spiro ring system with a dimidone unit has attracted widespread attention .Herein, we report the first direct synthesis of dispiro compounds including two Dimidone units.

2.Results And Discussion

Stereoselective reactions have appeared as synthetic tools for the formation of C─C and C─N bonds in aldol, Michael, Diels–Alder, Mannich, and relevant reactions , with high diastereoselectivity. In recent years,domino Knoevenagel/Diels–Alder reactions were reported for the diastereoselective synthesis of highly substituted spirotriones . The authors proposed a mechanism for the reaction that proceeds via a Knoevenagel condensation between 1,3-dicarbonyl compounds and aldehyde, followed by the Diels–Alder reaction of the aralkylidene 1,3-dicarbonyl with the in situ formed dieneamine through the reaction of the enone.

Previously, we developed our investigations on the basis of the synthesis of spiro compounds.Herein, we report a direct synthesis of dispiro [tetrahydroquinoline-bis(5,5-dimethylcyclohexane-1,3-dione)] derivatives in a diastereoselective manner at ambient temperature in acetic acid media. These compounds are produced through combinations of domino Knoevenagel, aldol,and Michael reactions.As shown in Scheme 1 and on the basis of the mechanism(Scheme 2), we suggest that the products are formed from the condensation of three equimolar dimidone, four equimolar aldehydes, and one equimolar aniline. To examine the efficiency and the applicability of this new domino multicomponent reaction, different aldehydes and arylamines were tested. Aromatic aldehydes bearing either electron-withdrawing functional groups, such as nitro and halo substituents, or electron-donating ones were converted into corresponding products with good yields. Also, we applied arylamines with eitherelectron-donating groups such as methoxy or electronwithdrawing groups.

The results are summarized in Table 1.

Entry	**Aldehyhe**	**Amine**	**Product**	**Yield**
1	benzaldehyde	Aniline	SNS-3	80
2	Nitro-Benzaldehyde	Aniline	SNS-5	73
3	Salicyladehyde	Aniline	SNS-7	81

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Conclusions:

In conclusion, we have developed the direct synthesis of dispiro [tetrahydroquinoline-bis(5,5-dimethylcyclohexane-1,3-dione)] derivatives at ambient temperature in acetic acid media. This reaction has advantages such as availability and cheapness of starting materials, mild condition, and easy work-up. The suggested mechanism has been supported in an especial manner through combinations of domino Knoevenagel, Michael, and Diels–Alder reactions. Products have been characterized by IR, mass, ^{1}H NMR, ^{13}C NMR spectroscopy.

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Analysis of ambient air quality Status of Latur City using different parameters

Annarao Maruti Chougule*[1] P. V kamble[2]
Head Dept.Of Industrial Chemistry, Dayanand Science College Latur
Sub Regional Officer Latur Maharashtra Pollution Control Board

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Abstract

This paper present ambient air quality status of latur city. There are three sites allotted in the region of study area which is residential, commercial and industrial,by Maharashtra pollution control board and Central pollution control board New Delhi, as per rules and regulation purpose to cover the entire area, the air quality was assessed based on measuring four air pollutants namely SO_2 (Oxides of sulfur), NO_x (Oxides of nitrogen) and RSPM (Respairable suspended particulate matter), SPM (Suspended particulate matter).The study of assessment period was one year from **January 2023 to December 2023** continuously two days (48 hours) per week, by operated Respairable dust sampler machine (RDS machine). After one year investigation the results found that the values of RSPM and SPM are beyond than the standards prescribed limit suggested by Central pollution control board (CPCB) in the area of residential and commercial. But amazingly it is observed that the RSPM and SPM below than the prescribed limit of CPCB in industrial site. The NO_X and SO_2 observed that all three sites are bellowing than the prescribed limit of CPCB, but when comparisons takes place in between three sites it is found that slightly higher in commercial area .

Keywords-RSPM, SPM, SO_2, NO_x Ambient air quality

1.Introduction

Air pollution is the impurity of air due to the presence of substances in the troposhphere that are harmful to the health of human and other living existence, air pollution caused by both man made activity and natural phenomena,air quality is closely related with earths climent and ecosystem As we know that the human being need to continuous supply of air to exist. Due to the air pollution the adverse effect on human health, pollution causes by mainly combustion of coal and gas oil, burning of fossil fuel like coal,wood, dry grass, manufacturing processes that emission dust and gases, also sulfur and nitrogen containing compounds contribution to ambient concentration, vehicular activity, traffic density and other organic and inorganic pollutants these all causes increases in RSPM ,SPM ,NO_X,SO_2 .Transportation is the major sources of air pollution in Latur city, the other potential sources being waste material shops, industrial operations, combustion of waste, juice shops, construction activities and natural contaminants .

2. Materials And Methods:

Latur is one of the well-known city which is situated on the Balaghat plateau it is famous for international trade, education hub, small scale industries, production of Tur dal and Edible oils. Total area of the city is 32.56 Km^2 and situated 636 meters above the mean sea level annual temperature range from 13 to 41^{0}C the highest temperature is recorded 45.8^{0}C and lowest is 6.9^{0}C the monsoon occurs in month of June to September. Three monitoring sites of steady area located at Dayanand Science college, Residential area and Commercial area at Bhalchandra Blood Bank Ganjgolai, Industrial area at Water supply project.

Assessment period carried out during the month of ***January 2023 to December 2023***. Under the National Ambient Air Quality Monitoring Project, sponsored by MPCB Mumbai and CPCB New Delhi, and run by Dayanand Education Society Latur. From May 2008.Measurement for SO_2 and NO_x Sample monitoring through Thermo electrically cooled gaseous sampling attachment to RDS machine which is commercially available. Frequency of Sample collection is of Four hours duration, machine works for two days at each site in week .Tetra chloro mercurateand Sodium arsenate are used as absorbing reagent for SO_2 and NO_x respectively. Collected samples are analyzed by spectrophotometrically Sistronics spectrophotometer 166, and method used West & Geake for SO_2 and Jacob & Hochheiser method for NO_x .Measurement of PM_{10} and SPM Monitored Sample collection and data analysis was carried out by using a commercially available Respirable dust sampler (RDS-Envirotech APM 411TE model).

Usually the air was drawn at a flow rate of 1.1 to1.2 m^3per minute. The air inside the sampler passed through a combination of cyclone separator and filter in two stages. At the first stage, the cyclone separator was used to collect the bigger particles (particles in the size range of 10 to 100 µm).The rest of the particulates in the size range of 2.5 to 10µm were collected over a previously dried and weighed glass micro fiber filters (Whatman GF/A,203*254 mm).RDS is operated continuously for two days. However filter paper and cyclone cup was replaced at interval of eight hours as per central pollution control board norms and conditions. Thus the collection inside the container attached with the cyclone separator could give the mass of $PM_{10\text{-}100}$ and the collection over the filter paper could represent the mass of PM_{10} (RSPM)).The loaded and unloaded filters were weighed after conditioning them in desiccators and oven. Finally, the SPM concentration was calculated.

Table 1. Monthly average concentration of RSPM (PM_{10}) in µg/m^3 at three sites

Month	Residential area	Commercial area	Industrial area
January	46	53	55
February	50	56	58
March	52	57	58
April	63	55	60
May	59	57	59.3
June	89	52	55
July	46	44	49
August	45	47	53
September	42	46	49
October	49	50	53
November	54.5	52	51
December	51	53	51

Table 2. Monthly average concentration of SPM in µg/m^3 at three sites

Month	Residential area	Commercial area	Industrial area
January	73.4	69.2	81.1
February	80.6	71.3	87
March	81.6	77.4	87.6
April	80.4	82.7	90.3
May	77.9	79.8	94.2

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June	74.4	76.91	80.1
July	64.89	67.14	66.8
August	69.9	68.5	73
September	67.1	65.37	67
October	71.3	72.7	77
November	77.1	80.1	76
December	74.8	76.3	73.9

Table 3. Monthly average concentration of SO_2 in µg/m^3 at three sites

Month	Residential area	Commercial area	Industrial area
January	9.0	8.0	5.8
February	9.8	9.0	6.2
March	9.8	8.0	6.8
April	7.8	8.0	7.6
May	9.4	8.0	7.2
June	8.3	8.0	6.7
July	7.5	7.2	6.8
August	7.7	7.8	7.0
September	7.1	7.4	7.0
October	7.3	7.0	7.0
November	7.2	8.3	7.0
December	8.3	9.0	8.5

Table 4. Monthly average concentration of NO_xµg/m^3 at three site

Month	Residential area	Commercial area	Industrial area
January	14	13	13.0
February	14	13	13.7
March	14.3	14	13.8
April	23.2	12	16.5
May	16.6	15	15.9
June	14.2	14	15.2
July	12.5	12.4	11.9
August	13.3	13.4	15.0
September	12.5	12.7	13.0
October	12.43	13.0	12.0
November	16.9	14.0	14.0
December	13.8	14.0	14.4

Table 5.Average concentration(µg/m^3) of different pollutants for yearly at three sites

Sampling sites	RSPM	SPM	SO_2	NO_x
Residential	54.1	73.1	10.4	14.7
Commercial	51.7	74.1	7.8	13.2
Industrial	54.6	80.0	6.8	14.0

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Table 6. National ambient air quality standards (Annual) for different parameters in (µg/m^3)

Sampling sites	RSPM	SPM	SO_2	NO_x
Residential	60	140	60	60
Commercial	60	140	60	60
Industrial	120	360	80	80

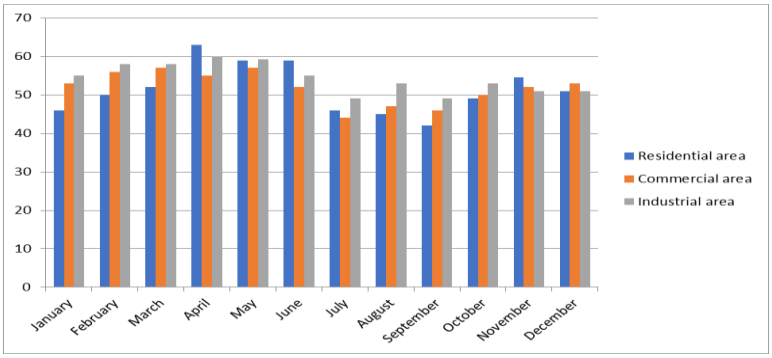

Fig.1 – Showing monthly average concentration of RSPM (µg/m^3) at Residential, Commercial, and Industrial area.

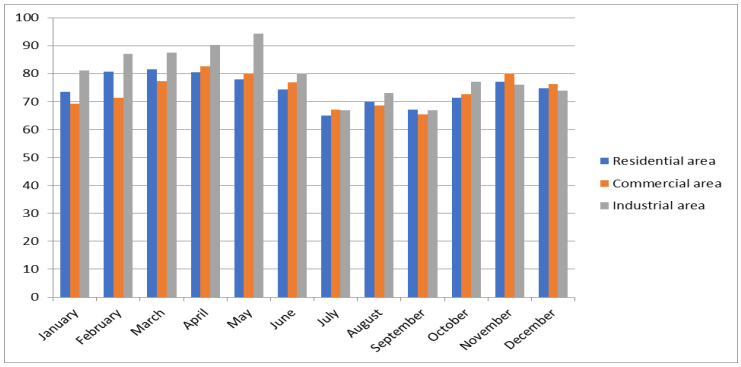

Fig.2 – Showing monthly average concentration of SPM (µg/m^3) at Residential, Commercial, and Industrial area.

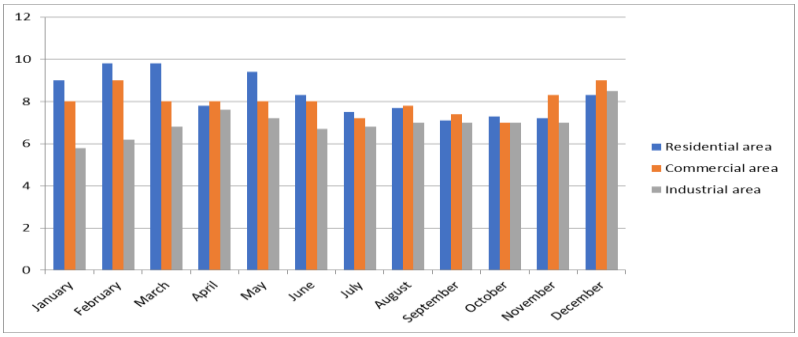

Fig.3 – Showing monthly average concentration of So2 (µg/m^3) at Residential, Commercial, and Industrial area.

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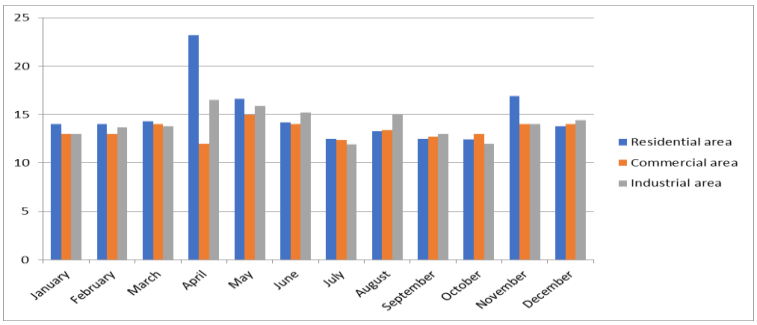

Fig.4 – Showing monthly average concentration of Nox (µg/m^3) at Residential, Commercial, and Industrial area.

Results And Discution

The statistical results RSPM for different sites have been presented in table 1.The observed minimum RSPM concentration was 42µg/m^3 and maximum was 68µg/m^3 at residential area. Minimum RSPM concentration was 49µg/m^3 and maximum was 71µg/m^3 at commercial area. Minimum RSPM concentration was 49µg/m^3 and maximum was 60µg/m^3 at industrial area. Average RSPM concentration was 58.1µg/m^3,59.8µg/m^3,54.6µg/m^3 at residential, commercial and Industrial areas respectively. From table 2.minimum SPM concentration was 68.7µg/m^3 and maximum was 91.1µg/m^3 at residential area. Minimum SPM concentration was 68.7µg/m^3 and maximum was 96.3µg/m^3 at commercial area. Minimum SPM concentration was 66.8µg/m^3 and maximum was 94.2µg/m^3 at industrial area. Averages concentration SPM was 80.2µg/m^3, 81.3µg/m^3 and 80.0µg/m^3 at residential, commercial and Industrial areas respectively. It was noticed that annual average concentration of RSPM and SPM at Residential as well as Commercial areas are above the National ambient air quality standards, because of not proper roads, school ground is near to Residential area, and short width roads, traffic density, waist material shops near commercial area. and it may be due to vehicular activity. Seasonal variations are also found at all sites. During the month of January to April it is maximum in Latur city and month of June to August it is found moderate and in the month of September to December it is again increases in the concentration of SPM, RSPM , SO_2 and NO_x at Residential and Commercial area. The reason may be increased October festival activity]. And in the industrial area there is not found any chemical industries so result of RSPM and SPM are below the prescribed limit. The Sulfur dioxide and Oxides of Nitrogen found from all three stations are normal in range shown in Table 3 and 4. But they were slightly increases in month of Dipawali festival.

Conclusion

The present investigation gives information about preliminary assessment of RSPM, SPM,SO_2 and NO_x concentrations. The average concentration of SO_2 and NO_x was bellowing the permissible limit of National ambient air quality standards, at three sites. The Average RSPM and SPM concentrations showed a variations and are higher in residential, commercial areas. In general transportation, abrasion process of automobiles, small-scale industries and elevated rate of combustion of convectional fuels are found to be the source of particulate pollutant in Latur city.

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An Analysis of the Water Characteristics of Beaches in And Around Mumbai Region, Maharashtra, India

Sanjay Shukla[1] Vipul Purohit[1]
[1]Department of Chemistry, Thakur College, Kandivali (E), Mumbai-400101;
Affiliated to University of Mumbai
vipulpurohit7@gmail.com

Abstract:

Beaches are a place to unwind in a city like Mumbai, where people lead hectic and stressful lives. Aside from this, the beaches' water serves a number of residential and commercial uses, including the fishing industry, which supports the country's economy. The state of the water has gotten worse as a result of human activity and the administration's careless attitude. Monitoring the water quality is crucial to improving this concerning situation. The current project entails the scientific collection of water from the several beaches in the Mumbai area, including Juhu, Gorai, and Manori Island. In order to determine how different seasonal variations affected the water quality, water samples were collected every three months. The estimate of several physico-chemical parameters that affect water quality is part of the current investigation. Electrical conductivity, total hardness, COD, DO, pH, color, alkalinity, and TDS are among the different parameters being examined. Chemical and instrumental approaches were used to test these characteristics. Different levels of contamination in different water bodies are the subject of the investigation. According to the data collected, some parameters were found to be beyond the WHO-established limit, putting aquatic life in jeopardy. In order to help the relevant authorities, take corrective action to enhance the quality of the water on these beaches, the current study takes a relative approach to the water quality from various locations.

Keywords: Aquatic life, chemical and instrumental procedures, physico-chemical parameters, and the fishing industry.

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1. Introduction

Since it is essential to the existence of humans, animals, and plants, water is one of the most valuable resources on Earth. Thus, "Water is Life." In addition to being used for drinking, water is also used for a number of other things, such as washing clothes and utensils, agriculture, the synthesis of numerous significant commercial items, and environmental cleansing and health maintenance.It is absolutely necessary that the drinking water be free of pollutants and pathogens that cause illness. Potable water is the term used to describe this pure water.The different water sources that are widely accessible are:
Water on the surface: In essence, this is the water that comes to the earth's surface as rain or hailstorms.The particular regions created for the purpose of gathering water are termed as catchment areas. Lakes and rivers: By enabling the movement of turbines, these bodies of water are typically utilized for irrigation. Additionally, these waters can be utilized to generate power at a low cost.

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The spring waters: This usually happens close to the lower part of a slope or sloping area where water naturally flows underground.Wells and bores: these are holes sunk deep into the earth to provide a steady supply of water.In order to make the water suitable for commercial use rather than drinking because it does not exceed WHO criteria, pipes are inserted into the hole and then forced towards the surface by high-pressure pumps. Water from these sources needs to be treated in order to be turned into drinkable water if it is unfit for human consumption.

Need of Study

Since the state of these waters eventually contributes to the healthy environment, it is crucial to check the quality of waters from these sources. The unsanitary activities of humans and animals, bathing and washing clothes, and the remnants of various religious rituals like flowers and the immersion of idols of various Gods and Goddesses pollute the waters of Mumbai's beaches. The following places are often where water quality monitoring is important: Human Health: Water is necessary for human consumption, and cholera, typhoid, and diarrhea are among the waterborne illnesses that can result from low water quality. Environmental Sustainability: Aquatic life, biodiversity, and ecosystem services can all be impacted by changes in water quality, which is a vital component of ecosystems. Economic Development: Agriculture, industry, and energy production all depend on water, and both food security and economic development can be impacted by low water quality. Recreational and Aesthetic Value: Poor water quality can affect the recreational, tourist, and aesthetic aspects that are frequently associated with water bodies. Implications of Low Water Quality:

Waterborne Diseases: Waterborne diseases, which can have serious negative effects on both health and the economy, can spread as a result of poor water quality. Degradation of the Environment: Reduced ecosystem services, habitat destruction, and biodiversity loss are all consequences of poor water quality. Economic Losses: Aside from effects on industry, tourism, and agriculture, poor water quality can also result in financial losses. Social and Cultural Effects: Human well-being, communal harmony, and cultural heritage are just a few of the social and cultural effects that poor water quality can have. Early Warning Systems and Water Quality Monitoring Benefits: Water quality monitoring can offer early warning systems for water pollution, enabling timely intervention to prevent or lessen effects. Better Water Management: Decisions on water management, such as the creation of efficient rules, policies, and management techniques, can be influenced by data from water quality monitoring.

Scope of Study

The evaluation of different water physico-chemical standards in relation to TDS, DO, pH, color, electrical conductivity, COD, and total hardness is the focus of the current study. Alkalinity using instrumental and chemical methods. Verifying these criteria and giving comparative statistics at the three beaches— Juhu, Gorai, and Manori —in Mumbai, Maharashtra State, India, are the tasks at hand.

2.Material and Methods

Water samples were collected from all the three locations quarterly i.e. at an interval of three months during the first week of April 24, July 24,October 24 and January 25. The American Public Health Association (APHA) and American Water Works Association (AWWA) standard procedures were used in evaluating the physico-chemical approaches. Different plastic, glass, and amber-colored bottles were utilized, depending on the criteria that needed to be assessed. The purpose of the pH meter was to measure the pH of different water samples. A TDS meter was used to measure TDS.The Winkler titrimetric method was used to determine DO.Ferrous

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ammonium sulfate and ferroin indicator were used to titrate the COD. Alkalinity was titrimetrically assessed, and total hardness was measured by omplexometric titration with Na-salt of EDTA in terms of ppm of CaCO3.A conductometer was used to measure electrical conductivity.The visual comparative method was used to determine the property of color.

3.Results and Discussion

The results obtained for the various parameters are presented in the following tables for the different samples from Manori Island labelled as M, Gorai labelled as G and Juhu labelled as J.

MONTH APRIL-2024

S.No.	Parameters	Units	Acceptable Limit	M	G	J
1	Temperature	^oC	-	28.0	27.5	27.2
2	pH	-	6.5-8.5	8.01	8.36	8.23
3	TDS	ppm	600	675	785	829
4	DO	Ppm	5	6.8	7.6	7.9
5	COD	Ppm	250	241	271	307
6	Total hardness	ppm	300	295	326	370
7	Alkalinity	ppm	200	215	278	312
8	Conductivity	S/m	5-50	48	58	66

MONTH July-2024

S. No.	Parameters	Units	Acceptable Limit	M	G	J
1	Temperature	^oC	-	27.0	27.2	26.8
2	pH	-	6.5-8.5	7.9	8.09	8.23
3	TDS	ppm	600	610	675	694

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4	DO	Ppm	5	6.2	7.4	4.3
5	COD	Ppm	250	229	264	310
6	Total hardness	ppm	300	320	346	382
7	Alkalinity	ppm	200	195	220	235
8	Conductivity	S/m	5-50	48	41	59

MONTH October-2024

S.No.	Parameters	Units	Acceptable Limit	M	G	J
1	Temperature	^oC	-	29.5	29.0	29.7
2	pH	-	6.5-8.5	7.21	7.56	7.83
3	TDS	ppm	600	595	635	695
4	DO	Ppm	5	5.4	6.6	7.1
5	COD	Ppm	250	256	288	306
6	Total hardness	ppm	300	305	348	380
7	Alkalinity	ppm	200	205	240	274
8	Conductivity	S/m	5-50	48	52	55

MONTH January2025

.No.	Parameters	Units	Acceptable Limit	M	G	J
1	Temperature	^oC	-	26.9	26.4	27.2

2	pH	-	6.5-8.5	7.91	8.11	8.22
3	TDS	ppm	600	612	669	694
4	DO	Ppm	5	5.8	6.6	7.25
5	COD	Ppm	250	244	278	326
6	Total hardness	ppm	300	295	314	338
7	Alkalinity	ppm	200	202	232	247
8	Conductivity	S/m	5-50	51	56	59

Conclusion

According to the data above, the values of the various parameters vary throughout the year depending on the temperature and climate as per seasonal changes. It can also be inferred that some of the parameters of the waters in all three of these locations are above the acceptable limits, necessitating the planning and implementation of a water treatment process. comparative studies show that the water quality at Juhu Beach is more polluted than at the other two beaches.

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Recent Advances and Future Perspectives in Spinel Ferrite Research: Synthesis, Characterization, and Applications

Jairam B. Mote
Corresponding author: jbmote51172@gmail.com
Department of Chemistry, Adarsh College, Omerga, Osmanabad, Maharashtra, India

Abstract

Spinel ferrites, a versatile class of magnetic materials with the general formula AB_2O_4 , have attracted significant research interest due to their unique combination of electrical, magnetic, and catalytic properties. Their wide-ranging applications in electronics, data storage, biomedicine, and energy technologies underscore their immense technological and industrial significance.

The historical development of spinel ferrites traces back to the early 20th century, with major breakthroughs in synthesis and applications emerging over the decades. The choice of synthesis method plays a crucial role in determining the structural, morphological, and magnetic properties of spinel ferrites. Conventional techniques such as solid-state reaction and wet chemical methods have evolved into advanced nano structuring approaches, enabling precise control over material properties. Characterization techniques, including X-ray diffraction (XRD), electron microscopy (TEM/SEM), and magnetic measurements (VSM, SQUID), are essential for understanding phase purity, microstructure, and magnetic behavior. Recent advances in spinel ferrite research have focused on tailoring their properties for enhanced performance in energy storage, environmental remediation, and biomedicine. However, challenges such as scalability, cost-effective synthesis, and stability under operational conditions remain key concerns. Future research directions emphasize optimizing synthesis techniques, developing multifunctional ferrites, and exploring new frontiers in quantum and spintronic applications.

This review provides a comprehensive analysis of the latest progress in spinel ferrites, highlighting their synthesis, characterization, applications, and future prospects. The insights presented herein aim to guide researchers toward addressing existing challenges and expanding the potential of spinel ferrites in advanced technological applications.

Keywords: Spinel Ferrites, Magnetic Materials, Synthesis, Characterization, Applications.

1. Introduction

Spinel ferrites are an essential class of magnetic materials, characterized by the general formula AB_2O_4, where A represents a divalent metal ion (such as Fe^{2+}, Ni^{2+}, Co^{2+}, or Zn^{2+}) and B represents a trivalent metal ion (typically Fe^{3+}). These materials have been widely explored due to their unique magnetic, electrical, and catalytic properties, making them crucial for various industrial and technological applications[1, 2]. Their adaptability, combined with tunable structural, optical, and electronic properties, has enabled their extensive use in multiple scientific disciplines, including electronics, medicine, energy storage, and environmental sciences.

The importance of spinel ferrites arises from their high thermal stability, excellent electrical insulation, moderate saturation magnetization, and tunable coercivity. These properties make them highly valuable for applications such as high-frequency inductors, transformers, magnetic recording media, spintronic devices, drug delivery systems, and catalysts for environmental remediation[3]. The

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ability to control their microstructure, composition, and performance characteristics through advanced synthesis and processing methods further enhances their potential for innovative applications[4].

This paper provides a comprehensive review of the recent advances and future directions in spinel ferrite research. It discusses various synthesis methods, their impact on structural and functional properties, and key characterization techniques that enable a deeper understanding of these materials. The paper also highlights the latest breakthroughs in spinel ferrite applications, the challenges associated with their development, and potential future research avenues aimed at optimizing their performance for next-generation technologies

2. Background and Significance of Spinel Ferrites

Spinel ferrites are a class of magnetic materials with the general formula AB_2O_4, where A represents a divalent metal ion (e.g., Fe^{2+}, Ni^{2+}, Co^{2+}, Zn^{2+}) and B represents a trivalent metal ion (usually Fe^{3+}). These materials are widely used due to their unique magnetic, electrical, and catalytic properties[5]. Their applications span from high-frequency electronics and biomedical imaging to energy storage and environmental remediation. The ability to tailor their properties through compositional modifications and synthesis techniques makes spinel ferrites highly versatile materials in both fundamental research and technological applications.

3. Historical Development of Spinel Ferrites

The study of ferrites dates back to the early 20th century when scientists discovered their unique magnetic behavior[6, 7]. The development of spinel ferrites gained momentum in the 1940s with the synthesis of commercial ferrites for use in transformers and inductors. Since then, advancements in materials science, nanotechnology, and characterization techniques have significantly enhanced our understanding of spinel ferrites, leading to their application in cutting-edge fields such as nanomedicine, spintronics, and catalysis.

4. Importance of Synthesis Methods

The properties of spinel ferrites are highly dependent on the synthesis method used. Various techniques, including[3]:

- **Solid-state reaction**: Traditional high-temperature synthesis, producing bulk ferrites with controlled stoichiometry[8].
- **Co-precipitation**: A low-temperature technique that enables the formation of nanosized ferrites.
- **Sol-gel synthesis**: A versatile method that allows for controlled particle size and morphology.
- **Hydrothermal and solvothermal methods**: These approaches facilitate the synthesis of highly crystalline ferrites with enhanced properties.
- **Green synthesis**: A sustainable approach utilizing plant extracts or biomolecules to produce ferrite nanoparticles with reduced environmental impact. Each method offers distinct advantages, influencing the structural, magnetic, and electrical properties of the resulting ferrites.

5. Role of Characterization Techniques

The thorough characterization of spinel ferrites is essential for understanding their structure-property relationships. Key characterization techniques include[9]:

- **X-ray diffraction (XRD)**: Determines the phase purity and crystallinity of ferrites.
- **Scanning electron microscopy (SEM) and transmission electron microscopy (TEM)**: Analyze morphology and particle size.

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- **Fourier-transform infrared spectroscopy (FTIR)**: Identifies functional groups and bonding characteristics.
- **Vibrating sample magnetometry (VSM) and SQUID magnetometry**: Measure magnetic properties such as saturation magnetization and coercivity.
- **X-ray photoelectron spectroscopy (XPS)**: Provides insights into oxidation states and electronic structure.
- **Impedance spectroscopy**: Evaluates electrical properties relevant to sensor and electronic applications.

6. Advances in Spinel Ferrite Research

Recent research has focused on:

- **Doping** strategies: Incorporating elements such as rare-earth metals to enhance magnetic and electrical properties.
- **Core-shell structures**: Engineering hybrid nanostructures for biomedical and catalytic applications.
- **Nanocomposites**: Combining ferrites with graphene, polymers, or other nanomaterials for multifunctional applications.
- **Spintronics applications**: Utilizing ferrites in memory devices and quantum computing.
- **Energy storage and conversion**: Application in lithium-ion batteries, supercapacitors, and water splitting.

7. Challenges and Future Directions

Despite significant progress, several challenges remain:

- **Scalability**: Developing cost-effective and scalable synthesis methods for industrial applications.
- **Stability**: Improving long-term stability in harsh environmental conditions.
- **Tunable properties**: Achieving precise control over magnetic and electrical properties.
- **Environmental impact**: Reducing the use of toxic chemicals in synthesis and enhancing recyclability.

Future research will likely focus on integrating artificial intelligence (AI) and machine learning for material design, exploring novel synthesis routes, and expanding applications in next-generation technologies[10].

8. Applications

Spinel ferrites have diverse applications in various fields:

- **Electronics**: Used in inductors, transformers, and microwave devices.
- **Biomedical field**: Magnetic resonance imaging (MRI) contrast agents, targeted drug delivery, and hyperthermia treatment.
- **Catalysis**: Used in environmental remediation, including wastewater treatment and CO_2 reduction.
- **Energy storage**: Applied in supercapacitors, lithium-ion batteries, and hydrogen evolution reactions.
- **Sensors and actuators**: Employed in gas sensors, biosensors, and electromagnetic wave absorption.

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9. Conclusions

Spinel ferrites are versatile materials with unique magnetic, electrical, and catalytic properties, making them valuable for various technological applications. Advancements in synthesis techniques have allowed for better control over structural and functional properties, enhancing their performance in different fields. Characterization techniques play a crucial role in understanding and optimizing ferrite materials for specific applications. Recent research has led to innovative developments such as doping strategies, core-shell structures, and nanocomposites that expand the utility of spinel ferrites. Despite their potential, challenges such as scalability, stability, and environmental concerns must be addressed for their widespread industrial adoption. Future research should focus on novel synthesis approaches, machine learning-driven material design, and further exploration of spinel ferrites in emerging fields like spintronics and energy storage. The continued development of spinel ferrites holds promise for significant contributions to next-generation technologies, from biomedical applications to sustainable energy solutions.

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Green Chemistry

Chate R. R.
Reddy P.S., Tirpude H.A.
Chemistry Department, PG students in Shivaji Mahavidyalya Udgir, (MH)-413517
Email:radhachate2017**@gmail.com**, reddypravin50@gmail.com

Abstract:

The object of Green Chemistry is the reduction of chemical pollutants flowing to the environment. The Chemistry and the Environmental Division has assumed Green Chemistry as one of its areas of interests, but one question to solve is where Green Chemistry should be placed within the context of Chemistry and Environment. The concept of Green Chemistry, as primarily conceived by Paul Anastas and John Warner, is commonly presented through the twelve principles of Green Chemistry. However, these Twelve principles through fruits of a great intuition and common sense, do not a clear connection between aims, concepts, and related research areas of Green Chemistry. The Twelve unsolved questions are the object of the present article.

Keywords: Green Chemistry's Principles, Pharmaceuticals, Sustainable Chemistry

1. Introduction:

Green chemistry, which is also commonly known as sustainable chemistry, is one of the aspectsof chemistry involving the design of products and processes that reduce or eliminate the use and/or generation of hazardous substances . A crucial aspect of green chemistry is the evaluation of the entire life cycle of a chemical product. This means evaluating not just the direct influence of the manufacturing process, but also the indirect environmental and health impacts in the usage and disposal phase. The use of natural resources and Environmental conservation should be well-balanced enough to address the situation effectively.The concept of "Green Chemistry" has acted to promote environmental conservationist awareness during the last 20 years. The novel laws and regulation that protect the ecosystem from harmful substances and designing new molecules with a This is a green chemistry strategy that diminishes the risk in human health and to the environment.

Definition Of Green Chemistry:

The Environmental Protection Agency (EPA) describes green chemistry as the field of chemistrythat produces chemical processes and products that prioritize environmental safety. The creation of chemical products should occur within a It is the manner through which, once their work isover, they are deconstructed to elements safe for the environment .

Evaluation Of Green Chemistry:

Industrialization developed world economic growth. Industrial activities improved the standardsof living, but international governments failed to regulate their effects on the environment. Excessive industrialization and food production caused pollution and exploitation of natural resources due to population increase. Natural resources were used without considering its environmental impacts. Environmental problems were first discussed and emphasized at the 1949 UNSCCUR in the US. It was at the 1968 Intergovernmental Conference of Experts on the Scientific Bases for Rational Use and Conservation of Biosphere Resources (Biosphere Conference) where environmental problems were once and for all brought to focus. The environmental movement had been triggered by "Silent Spring" in the 1960s. The historical book raised ecological awareness and urged government action to address natural resource overexploitation . Robert Downs called it "the book that changed America," while John Kenneth Galbraith referredto it as a major Western novel . Representatives from the UN and non-governmental organizations debated environmental law during the 1972 Stockholm Conference in Sweden17. After this conference, the world learned about ecosystem depletion's environmental risks. By the 1980s, there were several global environmental conferences. After analyzing 10 years of planned activities at the Stockholm Conference, the UN created the World Commission on Environment and Development in 1983 to report on global development and the environment. The group was formed amid global environmental pressure and knowledge of unsustainable development. The 1987 Brundtland Report, for the first time, combined environmental and socioeconomicconsiderations, to propose sustainable development, addressing current needs

without harming future generations. The study emphasizes ozone depletion and global warming risks threatening humankind, asserting that the experts cannot give remedies owing to the change in the speed of climate. In 1985, the OECD Environment Ministers decided on Economic Development and Environment, Pollution Prevention and Control, and Environmental. Information and National Reviews. These judgments lasted until 1990. These interventions were essential for minimizing chemical product danger and contamination . The 1991 US Environmental Protection Agency (EPA) "Alternative Synthetic Routes for Pollution Prevention" initiative stressed the significance of preventing harmful chemical compounds from being created. The program was renamed Green Chemistry in 1992 after adding safer and greener solvents. The 1990s world focus was on environmental protection. Brazil hosted the 1992 UN Conference on Environment and Development. Heads of state created Agenda 21, which commits countries to sustainable development through environmental, economic, and decision-making factors. Though environmental progress has been achieved worldwide, the environmental consciousness among corporations remains weak. According to Almeida, due to media and civil society pressure, corporations have only reluctantly followed government environmental regulations. In 68 countries, the 1984 Canadian initiative "Responsible Care" has transformed corporate behavior. This plan invested in infrastructure security, energy efficiency, employee safety records, and hazardous emissionreductions to improve quality of life and safety. The 1994 European Chemical Industry Council (CEFIC) study found that the public disliked the chemical industry, notwithstanding environmental issues in industrial and commercial sectors. Population focused on the pharmaceutical and plastics sectors due to perceived benefits (Pandey, 2015). Most interviewees didn't think the chemical sector prioritized sustainability. Oil, gas, power, wood, and paper were preferred over transportation, safety, and waste. In 1995, theUS government created the Presidential Green Chemistry Challenge (PGCC). Technological advances in the chemical sector reduced waste in various manufacturing areas. The works are honored annually in five categories: Academic, small company, alternative synthetic methods, reactive circumstances, and safer chemical designs are covered by Cann (1999). The non-profit Green Chemistry Institute (GCI) was created in 1997 to promote chemical company sustainability and green chemistry applications (ACS Chemistry, 2017). The GCI joined the ACS in 2001 to address global chemistry and environmental issues. Green chemistry research reached the industries, businesses, education, conferences, and international networks (ACS Chemistry, 2017). "Advanced with the 1998 book, Green Chemistry: Theory and Practise" by Paul Anastas and John C. Warner. The book focuses on academic and corporate environmental responsibility by the 12 Principles of Green Chemistry (ACS Chemistry, 2017). Rio + 10, the World Summit on Sustainable Development, took place in Johannesburg, South Africa, with thousands of attendees 30 years after Stockholm. Drawing on ECO-92 debates, government and non-governmental organizations, large enterprises, sectoral associations, delegations, and media discussed Agenda 21 government and public implementation alternatives. ACS Green Chemistry Institute (GCI) and international pharmaceutical companies held a panel discussion in 2005 to promote green chemistry and engineering in the pharmaceutical industry. Panelists believed "continuous processing" was necessary to "the green"; Constable, 2007). IUPAC, ACS, and GCI sponsored four Green Chemistry conferences between 1997 and 2011. Lenardão described the symposia as focusing on green goods, processes, energy sources, waste sources, policies, and education in green chemistry. The chemical and ecological engineering research has utilized sustainable methods. However, industrial processes and policies are required for environmental benefits.

Principles Of Green Chemistry:

The disappearance of harmful or dangerous compounds during the synthesis, manufacture, and application of chemical the products is covered in Poul Anastas' twelve principles of green chemistry. It is impossible to conceive a green chemistry process which fulfills all of the twelvecriteria at once, but attempts to do so during There exist different specific stages of synthesis.

Prevention: It is always good to prevent the generation of waste rather than the treatment orcleaning up afterit has been generated. precautions need to be taken to create no waste materials, than to clear the wastage after it is built.

Atom Economy: Good Synthetic methods should always be designed to maximize the utilization of all the reactants used in the process into the desired final product. New ways and methods should be created to incorporate each and every this is material used within several different processes that may prepare the final product.

Less Hazardous Synthesis: The synthesis procedures need to be designed as much as possible to use and produce less hazardous, not only to the health but to the surroundings**.**

Designing Safer reactants, solvents and other chemicals: The chemical substances should be designed in such a way that their desired function remains but in minimized quantityor with no toxicity.

Safer Solvents and Auxiliaries: The used quantity of solvents and other agents likeseparating agent's costs are higher so it's better to practice the safer one and reduce the unnecessary use.

Design for Energy Efficiency: As much as possible the synthetic methods should be developed to occur at ambient temperature and pressure in good yield. The use of high temperature as well as low temperature generates excess energy burden and the correlate problems.

Use of Renewable Feedstock: Whenever possible the use of renewable reagents, rawmaterials or feedstock's should be practiced.

Reduce Derivatives: The reduction of steps in synthesis will automatically use fewer reagents, less time, less energy and overall less risk, hazards and less generation of waste. So theunnecessary modification with using blocking groups, protecting and deprotecting groups, etc. should be reduced as much as possible.

Catalysis: The use of a proper catalyst will reduce the use of excess stoichiometric reagents soreduces ultimate waste and hazards

Degradable Design: They must be designed to degrade and transform into a non-toxic substance both to humans as well as to the environment. non-toxic chemical products must be developed and designed in order to enhance their functionality and create extremely low levels oftoxicity.

Real-time analysis for Pollution Prevention: Some analytical methodologies are developed and more is deemed to be developed further so we can observe at a real time that willprevent the generation of further hazards.

Inherently Safer Chemistry for Accident Prevention: Always we should keep in a mind should not use, or reduce the hazardous, explosive, recurrent accidents causing materials and replace it with a safer one that will minimize toxicity, prevent accidents, explosion, and fires.

Impacts of green chemistry: Currently the chemical-pharmaceutical industries and laboratories must contemplate green chemistry through, and not only, their analysis.

2 Advantages Of Green Chemistry:

1. Clean, fresh, and healthy air is released into the atmosphere which is clean air that is dangerous to the lungs to a lesser extent. It also decreases the air pollution caused due to suchenvironmentally friendly products.
2. Fresh water for drinking - sources of water to drink, like rivers, lakes, and ponds are protectedfrom pollution by non-hazardous chemical compounds not causing pollution. Contamination of water is also reduced with the reduction of the emission of hazardous material.
3. Workers' safety in the chemical industry is enhanced by use of non-accidental and nontoxic chemical materials. Also, workers do not encounter health complications due to prolonged exposure to hazardous chemicals; it's a saving grace for this industry.
4. Safer consumer goods - Consumers shall be offered safer and healthier options of goods that are being phased out.
5. The products will be free from pesticides and chemical cleaning agents, and will be prepared without producing much waste.
6. Foods will be made to stand longer before they become rotten because they will be healthier with more nutrition values and less likely to harbor bugs and worms.

3 Disadvantages of Green Chemistry :

1. This is the basic goal of green chemistry: designing chemical products and processes that reduce or eliminate harmful Substances. This objective is also the greatest of green chemistry that is reflected in time, costs and lack of information in specifically, converting from an old, traditional product to a

new "green" product, design of a new product and process is often not easy and quite expensive, no known alternative chemical or raw material inputs, also there is a lack of unity.
2. Weeds and pests can be dangerous since they may cross-pollinate with harmful genetically modified organisms.
3. Monoculture is used that requires large tracts of land which are often not available and which brings upon the farmers a Lots of sufferings.

4 Application Of Green Chemistry:

Pharmaceuticals: Design cleaner synthesis routes for pharmaceuticals; reduction of use ofhazardous solvents and reagents during drug manufacturing; greener waste disposal methods from pharmaceutical production activities.

Agrochemicals: Formulation of environmentally benign pesticides and fertilizers. Design of crop protection chemicals with lower ecological impact. Development of sustainable practices in agriculture to minimize chemical inputs. The application of green chemistry principles to agrochemicals is a way of making agricultural practices more sustainable and environmentally friendly in order to protect the health of ecosystems and improve the welfare of farmers as well as consumers.

5.Green chemistry in pharmaceutical industry: In the pharmaceutical industry, green chemistry plays an important role and makes a revolution in it. BASF, a chemical company now makes ibuprofen (painkiller) in a three-step rather than a six-step process. Zocor (simvastatin), leading drug for treating high cholesterol, conventionally synthesized using a multistep method concerning huge quantities of hazardous reagents that formed a big amount of toxic waste. A bio-catalysis company, Codexis developed a new synthesis route for the drug using a newly engineered enzyme and inexpensive feedstock. The chemotherapy drug, paclitaxel, marketed as Taxol, previously was obtained from yew tree bark through an extraction process in which huge amounts of the solvent were used in killing thetree. That tree cells are grown in a fermentation vat for the drug. Sonochemical method: In the last few years sonochemical method has developed for the preparation of materials. Ultrasonic irradiation (20 kHz to10 MHz) will always form acoustic cavitations. The primary concern with ultrasonic cavitations is in the formation, growth, and implosive collapse of the bubbles. The extreme conditions in these transient local hot spots include high temperature, pressure, and cooling rate which may offer an extreme environment for chemical reactions conditions. Chemical bonds are broken under such extreme condition and various material form through decomposition of volatile precursors within these rapidly collapsing bubbles. Sonochemical method applied on syntheses of drugs, dye etc., especially in combination with other sustainabletechnologies.

6.Application in nanoscience:

The nano materials have various applications in all disciplines. Researchers are working on the products of low dimensional materials, which are used in multi-purpose technical applications. Nanotechnology is also aware of our environment. Mechanical and chemical methods are developed for waste water treatment, air purification using nano filtration techniques. In recent years, green chemical approach is one of the important methods for synthesis of low dimensionalmaterials. Green chemical process deserves the merit pertaining to reducing agent choice, avoiding surfactants, solvent selection, and yield, particle size distribution, and purity. There are chemical synthetic methods that involve citrate method, tollens method, ionic liquid method, polysaccharide method, ligand exchanging method, polyoxometalate method in view of green chemistry. The reduction of gold salts by citrate anions was established some decades ago, and a nearly mono dispersed gold particles in nano range [29] . Synthesis of Ag nanoparticles using sucrose ester NaOH is added for the enhancement of the formation of silver nanosize Ag nanoparticles. Derivatives of carboxy methylcellulose (CMC) is used as a reducing agent to silver ions as well as for stabilizing while forming silver nanoparticles[30] . Industrial applications of green chemistry: Green Chemistry is not a lab-curiosity; instead it aims at big objective of creating a sustainable tomorrow. Increasing number of green methodologies developed by academic and industrial researchers enables companies to commer cialize these ideas. Industry, from small businesses to large corporations, has already made strategic moves towards sus tainability by adopting the principles of green chemistry. The development of less

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hazardous processes and commercial products, the shift from inefficient chemical routes towards biobased synthesis, and the replacement of oil-based feed stocks by renewable starting materials are only a few exam ples of the major decisions taken that will ultimately have vast consequences for the world chemical markets. As per the analysis of Environmental Protection Agency, the US drug industry has decreased the use of VOCs by 50% between 2004 and 2013 by adopting principles of green chemistry. In the same time span, the amount of chemical waste released to air, land and water decreased by 7% as per Toxics Release Inventory (TRI) of EPA. Recently four industrial drug units located in Hyderabad region of India has been closed on account of creating pollution. China, too, has strict environmen tal concerns and has taken regulatory action on 40% of the industrial units located in thirty provinces 32. These changes in policy suggest that it has become imperative to follow green practices. Plastics, in spite of several uses, have a bad reputa tion owing to their origin from polymers derived from non-renewable petrochemicals and their non-bio degradable nature. However, the same can be made from renewable feedstock as shown by a study carried out by Utrecht University 33. Studies byUtrecht Univer sity also show that the market of bio-plastics will grow by approximately 37% per year till 2013 and at a rate of 6% between 2013 and 2020. Many marketing hubs have joined the initiative to replace plastics with bio-plastics. Wal-Mart has been using bio-plastics in packaging wher ever possible 34. On similar lines Nokia, a mobile mak ing company, used 50% bio-plastics in Nokia 3111 Evolve phone cover as well as in Nokia C7 phone. 35 Using this technol ogy the yield increased from 50 to 98%. The Warner Babcock institute for Green Chemistry has developed a green hair-dye “Hairprint” which is a non toxic, vegetable-based product providing an alternative to the toxic, skin irritating and carcinogenic dyes.

Conclusion:

Green chemistry alone cannot solve the pressing environmental concerns and influences on our modern era but applying the twelve-principles of green chemistry into practice will finally help to pave the system to a world where the grass is greener The goal of green chemistry as mentioned early is based on twelve principles which aim to reduce harmful materials from the production, and application of chemical products. It is well known that when designing a green chemistry process, it is impossible to find the requirements of all twelve principles of the processat the same time. Nevertheless, it attempts to apply as many principles as possible during certain steps of synthesis. The goal of green chemistry in both environmental protection and economic gain can be achieved via many directions. For instance, chemical products would be prepared so that at the end of their function was not persist in the environment and instead break down into unhurt degradation products. As well as, the goals of green chemistry are as follows: to meet the wants of society in ways without harmful or depleting natural resources on earth which are the main objective of green chemistry. In this case, the focus is being shifted on manufacture products that can be fully reclaimed or re-used. Via changing patterns of production and consumption, steps are being taken to reduce pollution and waste, as one of the significant goals of green chemistry. It is critical to develop alternative technologies to prevent any further damage to health and the environment. It can be summarized that environmental conservation can be possible via the introduction of a green chemistry process.

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Synthesis of $MgFe_2O_4$ Nanoparticles via the Chemical Co-Precipitation route: XRD, FTIR, and VSM Characterization

[1]Shankar Dhanraj Birajdar*, [2]Ravindra C. Alange

[1]Department of Physics & Electronics, Dayanand Science College, Latur – 413 512, (M.S.), India
[2]Department of Physics & Electronics, Shri. Madhavrao Patil Mahavidyalaya, Murum., 413605, India
E-mail: *drshankarbirajdar@gmail.com

Abstract:

Magnesium ferrite ($MgFe_2O_4$) nanoparticles were successfully synthesized using a simple co-precipitation method. The structural properties of the synthesized nanoparticles were investigated using X-ray diffraction (XRD), which confirmed the formation of a single-phase spinel ferrite structure with high crystallinity. The average crystallite size was calculated to be approximately 22 nm using Scherrer's formula. The presence of metal-oxygen vibrations at tetrahedral (581 cm^{-1}) and octahedral (432 cm^{-1}) sites in the ferrite structure was confirmed by FTIR results. The M–H loop of $MgFe_2O_4$ was recorded using a Vibrating Sample Magnetometer (VSM), and magnetic parameters, including saturation magnetization (Ms), coercivity (Hc), and retentivity (Mr), were derived from the VSM data

Keywords: Nanoparticles, Magnetic, XRD

1. Introduction

The advancement of nanoscale science and engineering has brought a transformative shift in the field of materials, offering innovative techniques and applications across various disciplines. Nanomaterials are distinguished by their exceptional electrical, magnetic, and optical characteristics. Specifically, nanoscale ferrites possess outstanding electrical and magnetic properties, such as high electrical resistance, minimal dielectric losses, and strong saturation magnetization. These attributes make them highly effective for applications including energy and data storage, catalysis, sensing, magnetic resonance imaging contrast agents, and cutting-edge medical treatments [1]

Ferrites are composed of AB_2O_4 (where A = Cd, Co, Cu, Mg, Mn, Ni, Zn, and B = Fe) and typically crystallize in either a spinel or inverse spinel cubic structure, depending on the characteristics of the divalent cation A. In a "normal" spinel structure, A cations occupy tetrahedral sites, while trivalent B cations are positioned in octahedral sites. Conversely, in an inverse spinel structure, tetrahedral sites are occupied by B cations, whereas octahedral sites contain an equal distribution of A and B cations [2].

Among ferrites, magnesium-containing variants, such as $MgFe_2O_4$, adopt a cubic inverse spinel structure. These materials have garnered significant interest from researchers and the scientific community due to their outstanding properties and broad range of applications. Nanomagnetic magnesium ferrite is extensively utilized in a variety of technological fields, including biosensors, energy storage devices, hyperthermia treatment, heavy metal ion removal from wastewater, electrode material for lithium-ion batteries[5], degradation of organic pollutants, gas sensing, and textile dye removal. It is a magnetic bi-oxide ceramic with a partially inverse spinel structure. The cation distribution in magnesium ferrite can be represented as $(Mg_{1-x}^{2+}Fe_x^{3+})_a[Mg_x^{2+}Fe_{2-x}^{3+}]B\ O_4^{2-}$, where x indicates the degree of cation inversion within the lattice[3-5].

Researchers have developed several methods to synthesize nanomagnetic magnesium ferrite, including ultrasonic wave green synthesis, hydrothermal decomposition, supercritical hydrothermal reaction, micro-emulsion method etc. In this study, the chemical co precipitation was used to synthesize $MgFe_2O_4$ ferrite nanoparticles, and various physical properties, such as XRD, FTIR, and magnetic measurements, were Studied. The magnetic properties of the calcined powder (700 °C) were analysed using a vibrating sample magnetometer (VSM) with an SQUID-based magnetometer.

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2. Experimental

Pure magnesium ferrite ($MgFe_2O_4$) nanoparticles were synthesized using the chemical co-precipitation method. Ferric chloride hexahydrate ($FeCl_3.6H_2O$) and Magnesium chloride hexahydrate ($MgCl_2.6H_2O$) were dissolved in 100 mL of deionized water and stirred thoroughly. A 1 M sodium hydroxide (NaOH) solution was then added dropwise to adjust the pH to 14 while maintaining continuous stirring. The mixture was heated at 90°C for 4 hours until a brown precipitate formed. The precipitate was washed several times with deionized water and centrifuged to remove residual sodium hydroxide. The obtained product was first annealed at 80°C for 72 hours in a hot air oven. Finally, the samples were calcined at 700°C in a muffle furnace for 7 hours to attain $MgFe_2O_4$ nanoparticles with improved crystallinity.

The synthesized magnesium ferrite nanoparticles were analysed using various techniques for structural investigation. The crystal structure was examined via X-ray diffraction (XRD) using a Rigaku Mini flex 600 (Japan) with Cu-Kα radiation at 40 keV for phase determination. Fourier-transform infrared (FT-IR) spectra were recorded with a PerkinElmer spectrophotometer in the 400–4000 cm^{-1} range to confirm metal-oxide bonding in the material.

3. Result and Discussion

3.1 X-ray diffraction study (XRD)

Figure 1 presents the powder X-ray diffraction (XRD) pattern of Magnesium ferrite nanoparticles. The slightly broader peaks in the XRD pattern indicate a small crystallite size. All observed peaks correspond to the cubic spinel structure, confirming the formation of a single-phase sample. The average crystallite size was determined using Scherrer's formula from the broadening of the most intense (311) peak, yielding a value of 22 nm. The lattice constant 'a' was calculated using the following relation [6].

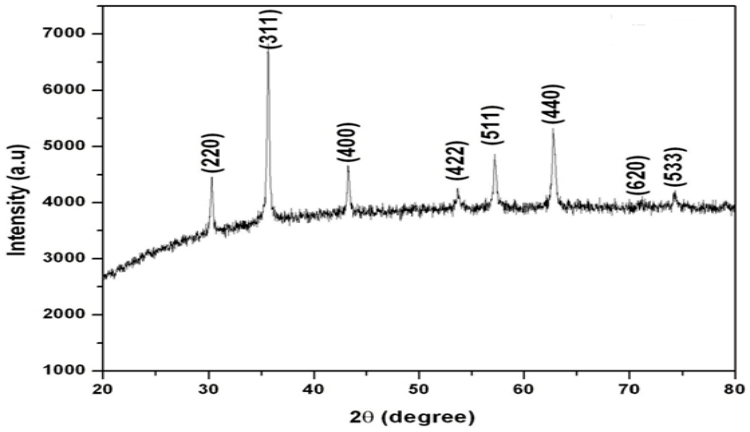

Fig. 1. X-ray diffraction patterns (Cu Ka -radiation) of MgFe2 O4 nanoparticles synthesized by the co-precipitation method

The lattice parameter 'a' was calculated using the relation:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

where h,k,l are the Miller indices of the crystal planes, and and d_{hkl} is the interplanar spacing. The lattice constant 8.36 Å obtained from XRD data falls within the reported range[7].

3.2 Fourier Transformed Infrared Spectroscopy Study (FTIR)

The FTIR spectrum of $MgFe_2O_4$ ferrite synthesized by the co-precipitation method is shown in Figure 2. FTIR analysis confirms the formation of the spinel ferrite structure. Two characteristic absorption bands are observed in $MgFe_2O_4$ spinel ferrite: a high-frequency band (ν_1) at 581 cm^{-1} and a low-frequency band (ν_2) at 432 cm^{-1}.

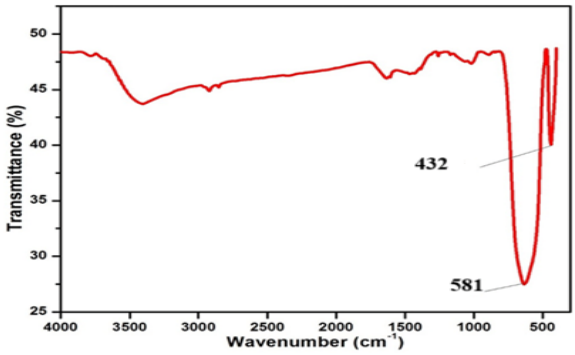

Fig 2. FTIR spectra of $MgFe_2O_4$ nanoparticles synthesized by the co-precipitation method

The high-frequency band (~600 cm^{-1}) corresponds to the intrinsic stretching vibrations of the spinel unit cell at tetrahedral sites (A), while the low-frequency band (~400 cm^{-1}) is attributed to metal-oxygen stretching vibrations at octahedral sites (B)[8]. This difference arises due to the shorter bond length of metal-oxygen bonds in tetrahedral sites and the longer bond length in octahedral sites. Additionally, absorption bands in the 1600–3400 cm^{-1} range indicate O–H stretching and bending vibrations, signifying the presence of free and absorbed water in the sample

3.3 Vibrating sample Magnetometer study (VSM)

The hysteresis loop is used to analyze the behavior of ferromagnetic materials in a magnetic field. Figure 3 presents the room-temperature hysteresis loop of $MgFe_2O_4$ synthesized via the co-precipitation method, confirming its soft magnetic nature.

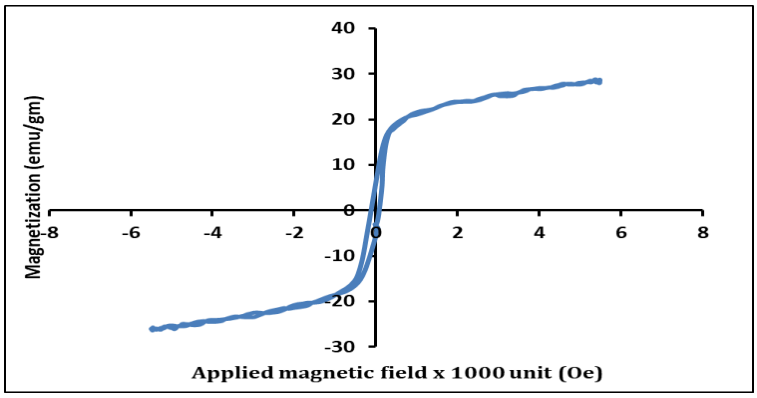

Fig.3 Hysteresis loop of MgFe2O4 nanoparticles at room temperature

The saturation magnetization (M_s), coercivity (Hc), retentivity (M_r), were determined from the curve as **27.98 emu/g, 1.567 Oe, 9.1829 emu/g, r**espectively. The sample exhibits a typical narrow (S-shaped) hysteresis loop, indicating a low coercivity value, which suggests that the material can be easily demagnetized [9]. Magnetic properties such as M_s, M_r, and Hc are influenced by factors like anisotropy density, grain growth, and A–B site exchange interactions. Smit and Wijn [10] reported a saturation magnetization value of **27 emu/g** for bulk $MgFe_2O_4$ particles, whereas the present sample shows a slightly lower value of **24.52 emu/g.** This difference can be attributed to variations in cation distribution, as changes in ion concentration and occupancy at A and B sites significantly affect the net magnetization.

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Coclusions

$MgFe_2O_4$ nanoparticles were successfully synthesized using the co-precipitation method and calcined at 700°C to improve crystallinity. XRD analysis confirmed the formation of a cubic spinel structure with a lattice constant of 8.36 Å, matching reported values. The average crystallite size, calculated using Scherrer's formula, was 22 nm, indicating nanoscale formation.FTIR spectroscopy revealed characteristic absorption bands at 581 cm^{-1} and 432 cm^{-1}, confirming metal-oxygen bonding in tetrahedral and octahedral sites, respectively.FTIR also detected O–H stretching and bending vibrations (1600–3400 cm^{-1}), indicating the presence of free and absorbed water in the sample's analysis showed soft magnetic behavior with a saturation magnetization (M_s) of 27.98 emu/g, low coercivity (Hc) of 1.567 Oe, and retentivity (M_r) of 9.1829 emu/g.The narrow (S-shaped) hysteresis loop confirmed the material's low coercivity, making it easily demagnetizable.Variations in magnetization values compared to bulk samples were attributed to differences in cation distribution at A and B sites. The synthesized $MgFe_2O_4$ nanoparticles exhibit promising properties for applications in magnetic storage, biosensors, catalysis, wastewater treatment, and biomedical applications

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DAYANAND COLLEGE OF PHARMACY

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Email: dayanandpharmacy@rediffmail.com

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DAYANAND INSTITUTE OF PHARMACY

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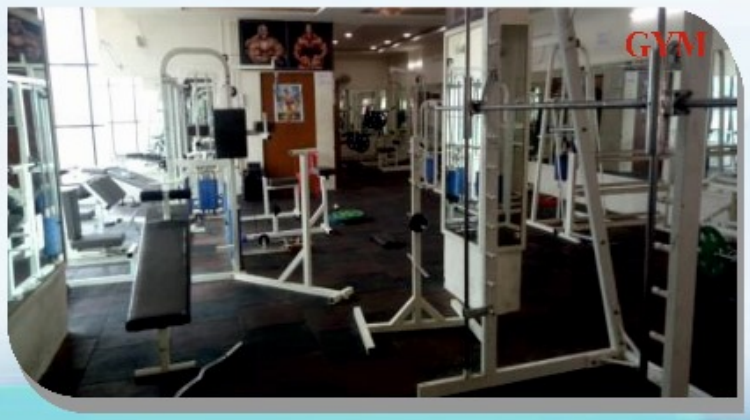

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