Two Day Virtual International Conference
on

CHEMICAL ADVANCES
for
SUSTAINABLE DEVELOPMENT

12th and 13th April 2022

Organised by
Department of Chemistry
University College for Women
Koti, Hyderabad

Department of Chemistry
University College of Women, OU, Koti

Editorial Board

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PROCEEDINGS

Two-Days Virtual
International Conference
on
"Chemical Advances for Sustainable Development (CASD-2022)"
12th and 13th April, 2022

DEPARTMENT OF CHEMISTRY
University College for Women (Autonomous)
Koti, Hyderabad-095

ISBN: 978-93-91576-87-5

sponsored by

TSCHE, Hyderabad

Two-Days Virtual International Conference on "Chemical Advances for Sustainable Development (CASD-2022)"

Conveners

Dr. G. Vijaya Lakshmi
1/c Head & Convener
Department of Chemistry
University College for Women
Koti, Hyderabad-095

Dr. V. Shashikala
Convener
Department of Chemistry
University College for Women
Koti, Hyderabad-095

DIVYA LAKSHMI PUBLISHERS DISTRIBUTORS

MEERUT

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Dr. V. SHASHIKALA
Convener
Department of Chemistry
University College for Women
Koti, Hyderabad-095

Published by

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Koti, Hyderabad-095

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Dr. B. Shailaja
Vice-Principal
University College for Women
Koti, Hyderabad-095

CONVENERS

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Koti, Hyderabad-095

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Mr. Rajagopal

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CONTENTS

	Page No.
1. Messages	1 – 14
2. Program Schedule	15 – 18
3. Speaker Profiles	19 – 29
4. Invited lecture Abstracts	30 – 35
5. Abstracts	36 – 90
6. Abstracts of Oral presentations	91– 149
7. Abstracts of Full Papers	151 – 158

MESSAGES

Telangana State Council Of Higher Education

(A Statutory Body of the Government of Telangana)
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Prof. R. Limbadri
CHAIRMAN

April 11' 2022

MESSAGE

Greetings from Telangana State Council of Higher Education!

At the outset, I congratulate Department of Chemistry, University College for Women, Koti for conducting 'Two Days Virtual International Conference on Chemical Advances for Sustainable Development (CASD-2022)" on 12th and 13th April 2022. It is informed that the Conference has received a huge response and it focuses on some of the key issues that is relevant for the future generations. The theme of the Conference indicates that chemical sciences play an important role in solving the major problems of the society in general and the world at large.

I appreciate the Organizing Committee for putting in their best efforts in conducting such a mammoth academic program, by going beyond the limits of regular curriculum. I am sure that such Conferences shall not only encourage the young minds towards novel research avenues but also inspires creativity and problem-solving skills among them.

I wish all the success to the team and hope that the deliberations of Conference will enrich the participants and benefit them.

I wish the Conference all success.

(PROF. R. LIMBADRI)

Prof. D. RAVINDER
Vice-Chancellor

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Estd. 1917
Reaccredited by NAAC with 'A+' Grade
University with Potential for Excellence
Category - I Graded Autonomy by UGC

April 08, 2022

MESSAGE

I am happy to learn that the Department of Chemistry, University College for Women, Koti, Osmania University is organizing a Two Day Virtual International Conference on "**Chemical Advances for Sustainable Development (CASD-2022)**" during April 12-13, 2022 and is bringing out Proceedings of the Conference to mark the occasion.

I compliment the Principal, Faculty, Staff and Students of the Department for their initiative in this regard.

The theme of the Conference is so timely and of topical significance. Today advances in Chemical sciences and its applications have occupied the centre stage of knowledge economy and hold key for the sustainable development of the society and in particular the country. Chemistry also enables more efficient use of our natural resources, increases energy efficiency, allows for reduced greenhouse gas emissions, finds new uses for current waste products, and is at the forefront of the development of sustainable materials.

I am sure this International Conference will provide a forum for deliberation on various issues pertaining to the theme and come out with useful policy inputs into the subject.

I wish the International Conference all success.

[PROF. D. RAVINDER]

Dr. P. LAXMINARAYANA
ME., Ph.D.
Professor of Mechanical Engineering &
REGISTRAR

(Re-Accredited by NAAC with 'A+' Grade)

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MESSAGE

I appreciate and congratulate the Department of Chemistry, University College for Women (O.U.), Koti, Hyderabad for conducting the "Two-day Virtual International Conference on Chemical Advances for Sustainable Development" between 12th – 13th April, 2022. I hope that this Conference will be useful to the participants in learning recent developments in Chemistry with special reference to sustainable development goals.

I wish the organizers and participants a very fruitful two days.

PROF. P. LAXMINARAYANA
REGISTRAR, O.U.

Prof. B. REDDYA NAIK
M.Sc., Ph.D.
OSD to Vice-Chancellor

Estd. 1917
Reaccredited by NAAC with 'A+' Grade
University with Potential for Excellence
Category - I Graded Autonomy by UGC

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MESSAGE

I am happy to know that Department of Chemistry, University College for Women, Koti, Hyderabad is organizing a Two Day Virtual International conference on Chemical Advances for Sustainable Development on 12th and 13th April, 2022 and bringing out a proceeding to mark the occasion. I hope the conference will certainly provide an excellent opportunity to the participants and delegates to interact with reputed speakers and update their knowledge in their thrust areas.

I congratulate the principal, faculty, researchers, scientists, students & participating industrialists for organizing such an innovative conference which is the need of the hour. Conference of this kind enables to integrate, synthesize, balance and accommodate knowledge from multiple functional areas in order to produce something greater than would be possible from any one disciplinary perspective.

I wish the conference a grand success.

Prof. B. REDDYA NAIK
OSD to VC

Prof. U. Umesh Kumar
Head

Department of Chemistry
University College of Science
OSMANIA UNIVERSITY
Hyderabad – 500 007, T.S, India.
Mobile: +919440567567
Email: utkoor@gmail.com

Date: 27/04/2020

MESSAGE

I am indeed delighted to note that, the Department of Chemistry, University College for Women, Koti, is organizing two days **Virtual International Conference on Chemical Advances for Sustainable Development CASD 2022** on April 12th and 13th 2022.

I believe that this international conference will give opportunities for sharing original research ideas and opinions, gaining inspiration for future research and broadening knowledge about various fields of Chemistry.

This conference will bring together research workers, scientists, academicians to a common platform so as to exchange ideas and stimulate discussions on recent advances in Chemistry.

I must congratulate the Principal, Head & Faculty of the department of Chemistry for taking up this responsibility and I am sure that this two days conference will be a grand success.

(Prof. U. Umesh Kumar)

Prof. P. Leelavathi
Chairperson, Board of Studies
Department of Chemistry

Osmania University
Hyderabad – 500 007.
Mobile : 9440621313
Email : leelaou@gmail.com

Message

I am pleased to know that the Department of Chemistry, University College for Women, Koti, is organizing a virtual international conference on "Chemical Advances for Sustainable Development" on 12th and 13th April, 2022.

The theme of the conference is quite relevant, timely as chemistry is at the forefront of the development of sustainable materials and hence the developments in this domain are to be understood and applied. I am sure that the planned conference will provide a right platform for young researchers and learners across the globe to share their knowledge and to interact with the experts in the area.

I compliment the Principal, I/c Head, staff, Department of Chemistry, UCW, Koti for their great initiative and efforts in designing the conference. I wish the seminar a great success.

Prof. M. Vijjulatha
Principal
University College for Women, OU, Koti Hyderabad

It gives me immense pleasure to present the proceeding of the Two Day Virtual International Conference on "Chemical advances for sustainable development" (CASD 2022). Sustainable development promises a better world, above all it pledges to leave no one behind. Responsible consumption and production are necessary in order not to endanger future generations, while respecting the earth's carrying capacity limits and universal human rights. Every country, every company and every one of us are affected by the consequences of climate changes. This international conference on chemical advances for sustainable development vitrines many eminent speakers and with technical sessions making it a vibrant platform that promotes the solutions for the sustainable developments.

The proceedings of CASD 2022 provides a glimpse of innovative ideas received from the Students, Research scholars, Scientists, Teachers, Innovators and Creative minds. I am hopeful that the event will encourage the young minds to come up with innovative ideas for transforming the world to be a better place through sustainable development.

Dr. B.Shailaja
Vice- Principal

Message

I am delighted to note that Department of Chemistry, University College for women, Koti, Hyderabad is hosting a two days Virtual International Conference on Chemical Advances for Sustainable Development on 12th and 13th April 2022, and bringing out the souvenir to commemorate the event. The chosen topic for the International Conference is most relevant and significant to the contemporary era. There was good response from practitioners, academia and research scholars who have actively responded and sent the research articles for all the themes and all sessions.

I would like to congratulate the Head, Department of Chemistry and also the organizing committee. I hope the conference would be very successful in the true and spirit. I wish Department of Chemistry all the success in conducting the conference.

(Dr.B.Shailaja)

MESSAGE by Dr. G. VIJAYA LAKSHMI, I/c Head, Department of Chemistry & Convenor, UCW

It gives me a great pleasure to conduct a Two-Days Virtual International Conference on "Chemical Advances for Sustainable Development (CASD-2022)" in the Department of Chemistry, University College for Women, Hyderabad.

We cannot imagine the world without chemical sciences and its applications. Chemistry is a Central Science which has been witnessing gradual and significant evolution over centuries. In the next fifteen to twenty years, when the world is going to face crucial situations, chemical sciences will be increasingly required to solve the world's greatest challenges.

Entropy of Universe is increasing and so are the global issues. There are major changes happening in science and society due to technological advancements. With this, new exciting opportunities are emerging with far-reaching implications for the future of the chemical sciences. The nature of chemistry research and chemistry careers need to be more diverse, inclusive, sustainable and environmentally benign. It becomes very imperative that novel research trends be created by the future generations and bring in more innovations for solving the world's problems. As a step in this direction, the Conference has been meticulously designed to address some of the key issues such as development of sustainable materials, providing clean energy, efficient use of natural resources and many more which are relevant in the present-day scenario. The massive response received through registrations stands as a testimony to the keen interest in the theme of the conference with more than 200 registrations, 78 oral presentations, 100 abstracts and 25 full papers. I hope that the discourses, deliberations and discussions apart from Technical Sessions planned in the Conference will enrich the academicians, research scholars and participants with the required knowledge and information.

In this context, I express my deep sense of gratitude to **Prof. M. Vijjulatha**, Principal, UCW and **Dr. B. Shailaja**, Vice-Principal, UCW for extending their kind support in all possible ways for the great success of the Conference. I am thankful to **Dr. V. Shashikala**, Convener, for extending immense cooperation for the successful conduct of the Program. I am extremely thankful to each and every Invited Guests and Speakers of all the sessions including Inaugural and Valedictory sessions and Evaluators of Technical Sessions for their tremendous contributions to the Conference making it more enriching, educational and worthwhile. I thank all the participants for their huge response, enthusiasm and timely response for making this program a successful event.

In a very special manner, I thank the Organizing Committee, faculty of Department of Chemistry, UCW for their unwavering support and immense contribution in making the program a grand success.

Dr. G. Vijaya Lakshmi
I/c Head & Convener
Department of Chemistry, UCW

"Development ..... without sustainability..... will leads to lethality....."

Dr. V. Shashikala, Convener
Assistant Professor
Department of Chemistry,
University College for Women, Koti,
Hyderabad, Telangana, India.

Sustainability is the utmost concern topic in the development of this Globe. In present situation of the Universe, I take this great opportunity to conduct two day virtual International conference on "Chemical Advances for Sustainable Development" on 12th and 13th of April 2022.

This conference is designed to learn from the research experiences, messages and views of eminent invited National and International guests, speakers. Technical sessions of this conference providing young researchers to express and share their novel thought of their research. The concept of cash prices for the best orals is to create a competitive spirit in bringing the best from the participants. I believe that the messages, lectures and sessions will give the road map for the importance of chemical advances for the sustainable development. And I am sure that all the participants will get benefit from this two day virtual international conference.

My sincere thanks to Prof. M. Vijjulatha, Principal, Dr. B. Shailaja, Vice Principal and Dr. G. Vijayalakshmi, I/c Head department of chemistry University College for Women, Koti, Hyderabad, and the organizing committee for their constant support in framing this conference. I sincerely thank to all the invited guests and speakers and evaluators giving their valuable time and all the participants for making this conference a big success.

Dr. V. Shashikala,
Convener

DEPARTMENT OF CHEMISTRY

UNIVERSITY COLLEGE FOR WOMEN, Koti, Hyderabad-095

Two Days Virtual International Conference

on

"CHEMICAL ADVANCES FOR SUSTAINABLE DEVELOPMENT (CASD 2022)"

Dates: 12th and 13th April 2022

PROGRAM SCHEDULE

Day – 1 Date: 12th April 2022, Tuesday

10.00 AM – 11.20 AM	INAUGURAL SESSION
10.00 AM – 10.05 AM	Welcoming the Guests
10.05 AM – 10.10 AM	Significance of the Conference – Dr. G. Vijaya Lakshmi, Convener & I/c Head, Department of Chemistry, UCW
10.10 AM – 10.15 AM	Message by Prof. M. Vijjulatha, Principal, UCW
10.15 AM – 10.20 AM	Message by Dr. B. Shailaja, Vice-Principal, UCW
10.20 AM – 10.30 AM	Message by Guest of Honour Prof. U. Umesh Kumar, Head, Department of Chemistry, University College for Science, Osmania University, Hyderabad

Profile by Dr. V. Shashikala, Asst. Professor, Dept. of Chemistry, UCW

10.30 AM – 10.45 AM	Message by Chief Guest Prof. Battu Satyanarayana, Hon'ble Vice-Honourable, Karnataka Central University, Karnataka

Profile by Dr. V. Shashikala, Asst. Professor, Dept. of Chemistry, UCW

10.45 AM – 11.15 AM	Message by Keynote Speaker Prof. Govardhan Mehta, Professor, FRS University Distinguished Professor & Dr. Kallam Anji Reddy Chair

Profile by Dr. K. Premalatha, Asst. Professor, Dept. of Chemistry, UCW

11.15 AM – 11.20 AM	Vote of Thanks by Dr. G. Vijaya Lakshmi, Asst. Professor, Department of Chemistry, UCW

Invited Lecture – I

Session Coordinator – **Dr. A. Swaroopa Rani,** Assistant Professor, Dept of Chemistry, UCW

11.20 AM – 12.00 PM

Prof. P. V. Anantha Lakshmi, Professor, Department of Chemistry, University College for Science, Osmania University, Hyderabad

Invited Lecture – II

Session Coordinator – **Dr. P. Mamtha,** Assistant Professor, Department of Chemistry, UCW

12.00 PM – 12.40 PM

Dr. B. Beeraiah, Associate Professor, Department of Chemistry, IIT Madras, Chennai.

Invited Lecture – III

Session Coordinator **– Dr. Aliya Begum,** Assistant Professor, Department of Chemistry, UCW

12.40 PM – 1.20 PM

Dr. Raghu Chitta, Department of Chemistry, NIT, Warangal, Telangana

Invited Lecture – IV

Session Coordinator – **Dr. N. Kavitha,** Assistant Professor, Department of Chemistry, UCW

1.20 PM – 2.00 PM

Prof. Ajay Kumar Mishra, Professor, Department of Chemistry, School of Applied Science, Kalinga Institute of Industrial Technology (KIIT) Deemed University, Bhubaneswar, Odisha.

2.00 PM – 2.15 PM LUNCH

Technical Session – I & II (Parallel Sessions) 2.15 PM – 4.30 PM

EVALUATORS

1. **Dr. A. Hari Padmasri,** Associate Professor, Department of Chemistry, UCS, OU
2. **Dr. M. Kavitha,** Assistant Professor, Department of Chemistry, UCS, OU

Session Coordinators:

a) **Dr. Ravikiran,** Department of Chemistry, UCW
b) **Mrs. J. Sowmya,** Department of Chemistry, UCW
c) **Dr. L. Yamini,** Department of Chemistry, UCW
d) **Mrs. P. Revathi**, Department of Chemistry, UCW

Two Days Virtual International Conference on

"CHEMICAL ADVANCES FOR SUSTAINABLE DEVELOPMENT (CASD 2022)"

Dates: 12th and 13th April 2022

PROGRAM SCHEDULE

Day – 2 **Date: 13th April 2022, Wednesday**

Invited Lecture – V

Session Coordinator – **Dr. S. Sreekanth,** Assistant Professor, Department of Chemistry, UCW

9.30 AM – 10.10 AM

Dr. G. Sudhakar Reddy, Smart Solutions USA Inc., University of Michigan Sustainable Coordinator.

Invited Lecture – VI

Session Coordinator – **Dr. M. Neelamma,** Assistant Professor, Department of Chemistry, UCW

10.10 AM – 10.50 AM

Dr. Addepalli Balasubramaniam, Rieveschl Laboratories for Mass Spectrometry, Department of Chemistry, University of Cincinnati, Cincinnati.

Invited Lecture – VII

Session Coordinator – **Dr. Ch. Sudhakar Reddy,** Assistant Professor, Department of Chemistry, UCW

10.50 AM – 11.30 AM

Dr. Radhakishan Motukuri, Senior Chemical Engineer / Material Scientist, Pacific Northwest National Laboratory, Richland, Washington, US.

Invited Lecture – VIII

Session Coordinator – **Dr. K. Ashwini,** Assistant Professor, Department of Chemistry, UCW

11.30 AM – 12.10 PM

Dr. Jayanthy Subbalakshmi, Associate Professor, BITS Pilani, Hyderabad Campus, Telangana

Technical Session – III & IV (Parallel Sessions) 12.10 PM – 1.40 PM

EVALUATORS

1. **Prof. G. Vijaya Charan,** Professor, Department of Chemistry, UCS, OU
2. **Prof. K. Girija Mangathayaru,** Professor, Department of Chemistry, Palamuru University, Telangana

Session Coordinators:

a) **Dr. E. Srivalli,** Department of Chemistry, UCW
b) **Dr. Ayub Shaik,** Department of Chemistry, UCW
c) **Mrs. Ameena Hussain,** Department of Chemistry, UCW
d) **Mrs. K. Narmada,** Department of Chemistry, UCS, OU

1.40 PM – 2.00 PM LUNCH

Invited Lecture – IX

Session Coordinator – **Mrs. J. Sowmya,** Assistant Professor, Department of Chemistry, UCW

2.00 PM – 2.40 PM

Prof. D. Basavaiah, Professor, School of Chemistry, University of Hyderabad, Hyderabad.

2.40 PM – 3.40 PM Technical Session continues

3.40 PM – 5.00 PM Valedictory Session

3.40 PM – 3.45 PM	Inviting the Guests
3.45 PM – 3.55 PM	Report on the International Conference by Convener
3.55 PM – 4.00 PM	Message by Principal, UCW
4.005 PM – 4.05 PM	Message by Vice-Principal, UCW
4.05 PM – 4.20 PM	Feedback from the participants
4.20 PM – 4.30 PM	Message by Guest of Honour Prof. P. Leelavathi, Chairperson, Board of Studies, Department of Chemistry, University College for Science, Osmania University, Hyderabad
4.30 PM – 4.40 PM	Message by Guest of Honour Prof. D. Ashok, BSR Fellow, Department of Chemistry, University College for Science, Osmania University, Hyderabad
4.40 PM – 4.55 PM	Message by Chief Guest Prof. D. Ravinder Sir, Hon'able Vice-Chancellor, Osmania University, Hyderabad.
4.55 PM – 5.00 PM	Vote of Thanks by Dr. V. Shashikala, Asst Professor, Department of Chemistry, UCW

PROFILES OF SPEAKERS

Prof. Goverdhan Mehta

Professor, FRS
University Distinguised Professor &
Dr. Kallam Anji Reddy Chair
School of Chemistry, University of Hyderabad.

Ph. D.	Poona University, 1967
Postdoctoral Research	The MSU and OSU, 1967 - 1969
Assistant Professor	IIT, Kanpur, 1970 - 1976
Professor	University of Hyderabad, 1977 – 1998
Vice-Chancellor	University of Hyderabad, 1994 - 1998
Director	IISc, 1998 - 2005
CSIR Bhatnagar Fellow	2005 - 2010
National Research Professor	2009 - 2014

Research Interests

- Chemical Sciences - Organic Chemistry (Synthesis).
- Design and reactivity of novel molecular objects and entities, total synthesis of complex bioactive natural products.
- Creation of NCE's for drug discovery, origin and control of stereogenesis
- Crystal engineering of conformationally locked polyols and photodynamic therapy of cancer.
- More recently involved in profiling and promoting chemical sciences as sustainability science

Prof P. V. Anantha Lakshmi , M.Sc (Inorganic Chemistry) (O.U), Ph.D (O.U) .

- Her academic qualification is MSc Chemistry (Inorganic), PhD.
- She has 29 yrs PG teaching experience, taught various topics at P G level, Compiled manuals for P G students, Established new courses
- She is resource person at Department of Chemistry, SKD University, MG University, APSWRJC and many colleges
- She received Dr Sabitha MLN Reddy Gold medal for being stood first in MSc Inorganic Chemistry during the academic year 1984-1986 CSIR Fellowship in 1987, Best teacher award by Chemical Research Society of India in 2011
- She did research on Synthesis, Structural Elucidation of Transition Metal Complexes Derived from some Biologically Active Quinoxaline Derivatives
- Her research areas are Coordination Chemistry, Drug DNA interactions, Synthetic Organic Chemistry, Pharmaceutical analysis, Drug polymorphism studies and impurity profiling of drug substances.
- Registered guide of Osmania University and IGNOU, Eight were awarded PhD, two submitted, four are persuing work.
- She has 58 published papers in National and International Journals to her credit and She is one of the authors in Intermediate First Year Chemistry Text Book and Intermediate Second Year Chemistry Text Book published by A.P. Telugu Academy, Telangana Telugu Academy.
- She is reviewer for Elsevier Journals like European Journal of Medicinal Chemistry, Wiley journals like Applied Organometallic Chemistry etc
- She completed four research Projects. 1. CPE minor research Project titled " synthesis of N-Heterocycles of biological importance by applying green methodologies" (2006-2007). 2. UGC Minor research project on "Synthesis and Characterization of Biologically active Transition Metal Complexes of Schiff bases derived from Hydrazino Quinoxalines" (2009-2011). 3. OU, DST-PURSE project on Synthesis, Characterization, DNA binding, cytotoxic and Anti-diabetic activity studies of metformin complexes (2018-2022) 4.UGC-CPE-FAR project on Transition metal complexes of Metformin: Synthesis, Structural, DNA Interaction and Anti-diabetic studies (2019-2020)
- Organised seminars / workshops

Served as

- Head, Department of Chemistry, UCW in 2014 & 2015
- Member, Board of Studies, Chemistry, University College for Women, 2008-2017
- Member, Board of Studies, Pharmaceutical Chemistry, Osmania University,2010-2012
- Member, U.G. Board of Studies, Chemistry, Osmania University, 2010-2015, 2019-2021
- Member, P.G. Board of Studies, Chemistry, Osmania University, 2013-2016
- Member, Departmental Committee, Department of Chemistry, OU, 2015-2017
- Coordinator, IQAC, UCW, 2016-2017
- Additional Controller of Examinations, Examination Branch, UCW 2007-2008
- Coordinator, Analytical Chemistry Course, University College for Women, 2011-2017.
- Coordinator, Quality Management Cell, University College of Technology, 2017-2018
- Involved in many confidential works

At present

- Member, P.G. Board of Studies, Chemistry, Osmania University & M.G.University.
- Member, Departmental Committee, Department of Chemistry, Osmania University
- Life member, Indian Council of Chemists and Indian Science Congress Association

Dr. Beeraiah Baire,
Associate Professor,
Department of Chemistry,
IIT Madras, Chennai

Ph.D. from IISc Bangalore (Prof. A. Srikrishna)

Postdoc: University of Minnesota, USA, (Prof. Thomas R Hoye)

Joined IIT Madras in Sept-2013, Currently Associate Professor

Research interests:

- ✓ Development of new synthetic strategies employing propargylic alcohols and derivatives as building blocks
- ✓ Total synthesis of Natural products and Drugs

Key Research developments:

1) The Z-enoate assisted Meyer-Schuster Rearrangement

2) A new *semi*-Favorskii rearrangement

3) The Hexadehydro Diels-Alder (HDDA) reaction for benzyne generation and reactions (during Postdoctoral research at Univ. of Minnesota)

PhD students: Graduated: 5; Current: 8

Research Publications: 69; patents: 1; Book chapters :2

Dr. Raghu Chitta
Assistant Professor,
Department of Chemistry
National Institute of Technology
Warangal

Professional Experience & Education

2018 – Present Assistant Professor, National Institute of Technology Warangal

2011 – 2018 Assistant Professor, Central University of Rajasthan

2011 (Jan) – 2011 (Jul) Post-doctoral Associate, Supervisor: Prof. Randolph P. Thummel, Professor, University of Houston, Houston, Texas, USA.

2007 – 2011 Post-doctoral Associate, Supervisors: Prof. Kent R. Mann, Prof. Wayne L. Gladfelter, Prof. Dr. David A. Blank, University of Minnesota, Twin Cities, MN, USA.

2002 – 2007 Ph.D., Research Advisor: Prof. Francis D'Souza Wichita State University, Wichita, KS, U.S.A. (Now at University of North Texas, Denton)

2000 – 2002 M.Sc., University of Hyderabad, Hyderabad, India.

1997 – 2000 B.Sc., Kakatiya University, Warangal, India.

Research Expertise: Artificial Photosynthesis, Photovoltaics, Water Oxidation, Fluorescent Molecular Probes

Ph.D. Guidance: Awarded 05

Research Publications: 47 (h-index: 32)

Patent: 1

Awards & Fellowships:

1. German Academic Exchange Service (DAAD) Fellowship for "Research Stays for University Academics and Scientists, 2016" under the supervision of Prof. med. Fabian Kiessling, RWTH, Aachen, Germany, 16th May – 15th July, 2016.

2. Summer Research Fellowship, Indian Academy of Sciences. Indian Institute of Chemical Technology (IICT), Hyderabad under the supervision of Drs. M. Lakshmi Kantam and L. Giribabu. June-July, 2014.

3. Recipient of the Dora Wallace Hodgson Outstanding Doctoral Dissertation Award at Wichita State University, Wichita, KS, United States

Prof. Ajay Kumar Mishra
Department of Chemistry,
School of Applied Sciences,
KIIT Deemed University, Bhubaneswar

Ajay Kumar Mishra (MSc, MPhil, PhD, CSci, FRSC) is currently working as Full Professor at the Department of Chemistry, School of Applied Sciences, KIIT Deemed University, Bhubaneswar, India. Professor Mishra is also affiliated as Director at the Academy of Nanotechnology and Waste Water Innovations, South Africa, Visiting Professor(s) at Robert Gordon University, UK, Bashkir State University, Russia, Vaal University of Technology, South Africa, Hebei University of Science and Technology, China and Adjunct Professor at Jiangsu University, China. Prof Mishra has been involved in the nanotechnology and waste water treatment projects. Active roles in these positions require Prof Mishra to visit annually, though not mandatory. These involvements have resulted in joint publications and joint supervision of master and doctoral students. Strategic projects have been designed for further joint project work. Prof Mishra's distinct educational and research background and hands-on experience have contributed to his emergence as a highly knowledgeable nano-scientists in the field. Prof Mishra completed his MPhil & PhD in Chemistry from the University of Delhi, India and obtained BSc & MSc in Chemistry from Purvanchal University (U.P. College), India.

Prof Mishra has published around 160 papers in peer-reviewed international journals and also represented in 150 or more papers in various conferences. He has edited more than 30 books and contributed over 65 book chapters in various peer reviewed edited books by established publishers. Prof Mishra has hosted many international visiting researchers and visited several universities globally. He has successfully graduated 13 PhD's, 20 Master's students of which mostly graduated cum laude (more than 75%), and hosted around 10 postdoctoral fellows. Prof Mishra's research has been cited more than 8200 times as per google scholar, with h-factor of 39. This is an additional testimony to his significant contributions to nanoscience & nanotechnology. Prof Mishra's salient and influential research virtually guarantees that it will continue to improve in the field of nanoscience & nanotechnology and produce high quality work. Recently, Prof Mishra have been named on a list of the top 2% of the most-cited scientists in various disciplines globally (2019-2021). Based on data from Elsevier's Scopus, the abstract and citation database, the report was prepared by Professor John Ioannidis of Stanford University and his team and published in the journal PLOS Biology Prof Mishra is also reviewers of several key peer-reviewed international journals besides active role as an external examiner for national and international Masters/PhD students. Prof Mishra has also secured number of international grants. Prof Mishra have attained considerable national and international recognition, as well as awards including "Fellow member" and "Chartered Scientist" by Royal Society of Chemistry, UK and Chancellor's Prize (Unisa) for excellent achievement in research. Prof. Mishra also served as Associate Editor as well as member of the editorial board of many peer-reviewed international journals and books. He is serving as member advisory board of a number of international scientific societies, conferences and workshops

Dr. Sudhakar Reddy

Email: redv@umich.edu

Dr. Sudhakar Reddy obtained his B.Sc in 1973, M.Sc from Osmania Univ in 1975, Ph. D. from National Chemical Laboratory, Pune in 1980 in the field of Mass Spectrometry and migrated to USA as a NASA post-doctoral fellow in 1981. After a few years of performing research at the Utah State University he worked as a Lab Manager for 7 years in the Shrader Analytical Lab in Detroit, Michigan and then accepted a position of Lab Director to join the University of Michigan in 1994 and worked there for 24 years in various positions, including his position as Campus Sustainability Coordinator. Dr. Reddy's contributions:

- Set-up a testing lab to measure priority pollutants at trace levels in air, water and soil
- Developed micro-scale and automated methodologies to reduce waste generation
- Promoted Green Chemistry and Engineering across the University of Michigan campus
- Architected and developed a unique Sustainable Lab program to save on energy, utilities and materials while promoting Green Chemistry leading to safer working conditions
- Trained and organized many workshops and conferences on Green Chemistry

Dr. Reddy was appointed by the Governor of Michigan to a Green Chemistry Round Table where he contributed to promote Green Chemistry at state level among higher educational institutions, including the University of Michigan. He has published 35 peer reviewed articles in the various international scientific journals/magazines and presented several invited talks and key note speeches in USA, UK, Kuwait, Singapore and India. Dr. Reddy was recognized for his contributions with numerous awards and rewards. A few prominent ones to represent as follows:

- Gold Medal recipient in Special B.Sc in 1973
- 2013: Governor of Michigan Green Up award on Green Chemistry
- 2014: Laboratory Sustainability award by the International Institute for Sustainable Labs (I2SL), USA
- 2015: Environmental Improvement award by S-Lab, United Kingdom

Dr. Reddy has retired in 2018 from the University of Michigan after 24 years of service. He is currently serving on many boards of professional, profit and non-profit organizations and provide consultation on Green Chemistry and Sustainability in lab operations.

Prof. Addepalli Balasubramaniam

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows, as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
Agricultural College, Bapatla, Andhra Pradesh, India	B.Sc.	06/1988	Agricultural Sciences
Indian Agricultural Research Institute, Delhi, India	M.S.	08/1990	Biochemistry
Indian Agricultural Research Institute, Delhi, Indi	Ph.D.	10/1994	Biochemistry
Department of Plant and Soil Sciences, University of Kentucky, Lexington, KY	Postdoctoral	12/2007	Biochemistry
CCTS, University of Cincinnati College of Medicine, Cincinnati, OH	Certificate	08/2013	Clinical and Translational Research

Previous position: Scientist, Indian Agricultural Research Institute, Delhi.

Current POSITION TITLE: Associate Professor

Research profile

My research focuses on unraveling the biological significance of chemical modifications to biomolecules (nucleic acids and proteins), and assessment of the use of protein and RNA therapeutics in resolving the biomolecular defects. My laboratory develops innovative and sensitive detection approaches such as liquid chromatography coupled with mass spectrometry (LC-MS) to identify and measure the levels of chemical modifications in cellular RNA, proteins, and impurities in the phosphorothioate oligonucleotide therapeutics. The chemical modifications include enzymatic (natural) and nonenzymatic (xenobiotic) changes to DNA, RNA, and proteins from a variety of biological systems. My group has developed sample preparation and LC-MS methods to detect post-translational modifications such as disulfide linkage, isoaspartate changes in proteins. Our current research also includes identification of post-transcriptional modifications (PTMs) that are susceptible to UVA-induced photooxidative damage and degradation. We have developed LC-MS methods for quantification of oxidized nucleic acids (including 8-oxo-dG and 8-oxo-rG for DNA and RNA, respectively), and protein peroxidation as a measure of the extent of UVR-induced photoproduct production.

Dr. Radha Kishan Motkuri

Senior Principal Scientist & Team Lead
Applied Chemistry and Engineering, Pacific Northwest National Laboratory
902 Battelle Boulevard, P.O. Box 999, MSIN K4-18
Richland, WA 99354 USA , Tel: 509-371-6484; Fax: 509-371-7249

Radha Kishan Motkuri, PhD, is a senior chemical engineer/material scientist with Pacific Northwest National Laboratory (PNNL). Dr. Motkuri has over 23 years of experience in inorganic and materials chemistry with an emphasis on nanoporous materials. More specifically, his work has focused on nanoporous materials including metal-organic frameworks (MOFs), covalent organic frameworks, covalent organic polymers, porous aromatic frameworks, hierarchical porous carbons, zeolites, and mesoporous silica for potential applications including sorption/capture, separation, catalysis, detection, and sensing.

Motkuri's research on nanoporous materials for potential applications, including adsorption cooling/refrigeration using fluorocarbons and water, is disseminated through various publications, patents, and awards. He was integral to developing thermal vapor-compression technology that runs off any low-grade heat source, called MARCool, for which he received a 2017 R&D 100 Award. His research for the AirJoule Self-Regenerating Dehumidifier—a heating, ventilation, and air conditioning component that recycles the heat it generates by removing water from the air—is also widely recognized and was awared as a 2021 R&D 100 Bronze award.

Motkuri and his team are currently developing two technologies to help locate and clean up hazardous perfluoroalkyl and polyfluoroalkyl substances (PFAS): a sensitive, portable sensor to detect PFAS in the field, and an innovative technology to capture PFAS. The latter could aid cleanup efforts aimed at protecting groundwater to help protect communities and ecosystems from PFAS. The fast PFAS sensor work was selected as a 2021 R&D 100 Finalist.

Motkuri earned his PhD in chemistry from the University of Hyderabad, dealing with nanoporous materials for supramolecular chemistry and catalysis applications. After he completed his Alexander von Humboldt fellowship on rotaxanes and supramolecular chemistry, he finished his postdoctoral research on molecular motors and boron chemistry.

RESEARCH INTERESTS

- Engineering of nanoporous materials
- Nanoporous materials for heating/cooling, adsorption chiller, dehumidification, power generation, direct air capture, and carbon capture applications
- Water purification, contaminant sensing and removal
- PFAS remediation including capture, sensing, and destruction
- Gas, vapor adsorption and separation
- Carbon sequestration
- Heterogeneous catalysis using nanoporous materials
- Novel synthetic methodologies for MOF synthesis
- Continuous and bulk production of MOFs
- Graphene and graphene oxide materials
- Chemical security, nuclear security, and energy security
- Supramolecular chemistry and nanotechnology

Prof. Jayanty Subbalakshmi

BITS-Pilani, Hyderabad

Prof. Jayanty Subbalakshmi completed M.Sc in 1997 with distinction, specialization in Physical Chemistry from Andhra University. She received her M.Phil degree in 1998 and Ph.D. degree in 2004 from the School of Chemistry, the University of Hyderabad under the supervision of Prof. T.P.Radhakrishnan. After completion of Ph.D., she moved to the Research Institute of Electronic Sciences (RIES), University of Hokkaido for postdoctoral study, as a JSPS fellow funded by the Japan Society for Promotion of Science. She joined BITS-Pilani, Hyderabad Campus in 2009 as a lecturer and very soon promoted in November 2009 as Assistant Professor, later to Associate Professor in 2015. She is a recipient of best research award in 2004 given by Dr. K.V. Rao Scientific Society. She received Distinguished Women in Science award (Major area of study: Chemistry) in 2019. She has over 35 publications in the reputed international journals. She filed overall three patents as a principal inventor, of which recently one patent is granted in November 2021, and two are under examination. A couple of her works recognized and received best poster awards in various international conferences. She has contributed a book chapter in the "Synthesis and characterization of templated polyanilines: A new class of polymeric materials: Functionalized Engineering Materials and Their Applications Apple Academic Press, CRC, Taylor and Francis Group. She completed two major DST funded projects as a principal investigator and currently two proposals are under review. Her research interests are in the design, synthesis, characterization and application of small organic molecules based on D-□-Acceptors such as tetracyanoquinodimethane (TCNQ), tetrathiafulvalene (TTF) and xanthenes for molecular material and biological applications. She is a life member of several scientific societies like Indian JSPS Alumni Association (IJAA)"Chemical Research Society of India (CRSI)", "Material Research Society of India (MRSI)", "Society Materials Chemistry (SMC)", by Bhabha Atomic Research Center, BARC Mumbai. She is currently guiding five Ph.D research scholars. She has guided several first degree thesis students and project students at BITS-Hyderabad. She is a member of Judges in the KVRSS. At BITS-Hyderabad she has been Convener of Doctoral Research Committee, Member of Academic Research Division and various others

Deevi Basavaiah

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Date of birth : August 11, 1950 **Nationality** :Indian

Education

- Postdoctoral Fellow (August 1980 – November 1983) at Department of Chemistry, Purdue University, West Lafayette USA (with Professor Herbert C. Brown, 1979 Nobel laureate in chemistry)
- PhD (1979) in Organic Chemistry, Banaras Hindu University (BHU), Varanasi-221 005 (India) (Research Supervisor : Professor Gurbakhsh Singh)
- MSc (1972) in Chemistry (Organic Chemistry) Banaras Hindu University (BHU), Varanasi-221 005 (India)
- BSc (1970) with Chemistry, Physics, Mathematics (Andhra Loyola College, Vijayawada) Andhra University

Professional details

- Scientist C : National Chemical Laboratory, Pune : January 1984-June 1984
- Lecturer : School of Chemistry, University of Hyderabad : June 1984-February 1987
- Reader : School of Chemistry, University of Hyderabad : February 1987-August 1996
- Professor : School of Chemistry, University of Hyderabad : August 1996-present

Awards and Honors:

i. Appointed as Honorary Professor at Chemistry Department, BHU, Varanasi for a period of three years i.e Jan. 2014-Dec. 2016.
ii. Awarded BHU Distinguished Alumnus Award - 2012
iii. INSA- Professor T. R. Seshadri 70th Birthday Commemoration Medal-2009
iv. The Indian Science Congress Platinum Jubilee lecture award in Chemical Sciences - 2009
v. National Best Teacher award in Chemistry 2008 (sponsored by A.V. Rama Rao Research Foundation in association with IICT and AP Academy of Sciences)
vi. J. C. Bose Fellowship (DST-New Delhi) -2008
vii. CRSI Silver Medal-2008
viii. Elected Fellow of the Indian National Science Academy (FNA)- 2006
ix. CRSI Bronze Medal- 2000
x. Professor T. R. Govindachari 60th Birthday Commemoration Endowment Award in Organic Chemistry 1999-2000
xi. Elected Fellow of the Indian Academy of Sciences (FASc) Bangalore -1997
xii. First Rank in M. Sc. Chemistry, Awarded B. H. U. Gold Medal- 1972
xiii. Awarded A. P. National Scholarship on the Merit of B. Sc. Marks- 1970

Main Field of Research Interests: Organic Chemistry
Specialization:1). The Baylis-Hillman Reaction 2). Chiral Catalysis
Total Publications :153; Ph.D.s guided : 38; Number of Ph.D. students working : 3

ABSTRACTS OF INVITED LECTURES

Engineered Nanoporous Materials for Potential Environmental Applications

Dr. Radha Kishan Motkuri

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Per- and polyfluoroalkyl substances (PFAS) are among the most abundant environmental contaminant species. They are widespread due to uncontrolled industrial and commercial use and have been linked to health risks such as cancer. With rising global concerns about the public health effects of PFAS, there is an incentive to develop strategies for reliable monitoring and effective PFAS removal, particularly in drinking water. This presentation is about our PNNL's unique strategies for PFAS sensing and removal with capture probe technology that has an affinity for fluorocarbons, including PFAS.

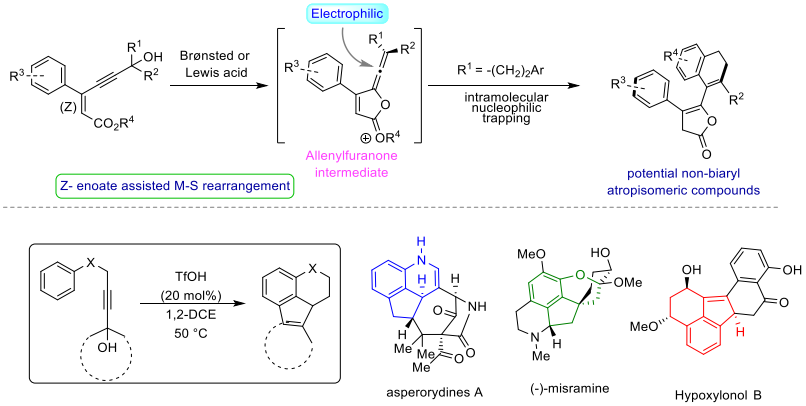
An acid Catalyzed Cascade reactions for Rapid Generation of Complexity

Dr. Beeraiah Baire,

Associate Professor, Department of Chemistry, IIT Madras, Chennai-36.

Email: beeru@iitm.ac.in

Cascade (domino) reactions are ideal techniques in organic synthesis for assembling complex structures within a faster timeframe.[1] Most of the time, these approaches provide mild reaction conditions thereby imparting a high tolerance for many functional groups. Polycyclic systems both carbocycles as well as heterocycles are important structural motifs found in a wide range of natural products and pharmaceuticals. Domino processes are very important and useful for the construction of polycyclic systems as they lead to the formation of many C-C and C-X bonds simultaneously. Propargylic alcohols and their derivatives are one of the most useful building blocks with two functional groups. These units have been employed in numerous cascade synthetic transformations in organic chemistry providing an opportunity to discover novel cascade processes.[2] In our laboratory we design and develop novel strategies based on acid catalysis employing propargylic alcohol derivatives as building blocks. The details of some our latest discoveries and developments in this area will be discussed in the presentation.



Scheme 1: Representative examples of an acid catalyzed domino reactions developed in our laboratory

References:

1. S. E. Denmark and G. A. Hite, *Helv. Chim. Acta*, **1988**, *71*, 195–208.
2. N. Pedireddi, R, V, Bokka, and S, Gedu, *ACS Omega*. **2018,** *3*, 218−228.
3. a) P. Tharra, B. Baire, *Chem. Commun*. **2016**, *52*, 12147-12150; b) P. Tharra, B. Baire, *Chem. Commun*. **2016**, *52*, 12147-12150; c) P. Tharra, B. Baire, *Chem. Eur. J.* **2017**, *23*, 2014-2017; d) B. Yadav, B. Baire, *Chem. Commun.* **2021**, *57*, 12796-12799.
4. a) L. F. Tietze, *Chem. Rev.,* **1996**, *96*, 115; b) K. C. Nicolaou, D. J. Edmonds and P. G. Bulger, *Angew. Chem., Int. Ed.,* **2006**, *45*, 7134; c) SK. C. Nicolaou and J. S. Chen, *Chem. Soc. Rev.,* **2009**, *38*, 2993. a) B. Alcaide, P. Almendros, M. T. Quirs, R. Lopez, M. I. Menndez and A. Sochacka-C'wikła, *J. Am. Chem. Soc.,* **2013**, *135*, 898; b) R. Chinchilla and N. Carman, *Chem. Soc. Rev.,* **2011**, *40*, 5084.

Nano-engineered Composite Materials for Environmental Sustainability

Ajay Kumar Mishra[1,2,3] and Shivani B. Mishra[2,3]

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Nanotechnology has been an emerging area of research due to its versatile applications in many research areas. Composite comprise of mixing two component where one is matrix and other one is reinforce materials. The reinforce materials based on their nano sizes results in nanocomposite materials. The nanocomposite materials usually possess a high surface area which ultimately enables in the remediation of waste water. Engineering of such composite/nanocomposite materials directly relates to enhance materials properties for various applications in the respective areas. Waste water remediation usually possess variety of area and our research mainly focusses on the removal of organic and inorganic components from the waste water. The current talk will be focused on the past, present and future scenario of nano-engineered composite materials for environmental sustainability.

An Introduction to the Green Chemistry Leading to Sustainability Development in the Learning and Teaching Methods

SUDHAKAR G REDDY, Ph. D.

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Green Chemistry can be defined as a design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. It also demands for safer working conditions while saving on operational costs, making it sustainable, thus calling it as Sustainable Chemistry. Although the concept of Green Chemistry is known to the chemical community in early nineties, a clear concept was developed by Drs. John Warner and Paul Anastas in 1998 through 12 Green Chemistry principals. These two educators are now referred to as Fathers of Green Chemistry. With a clear definition on this emerging area of sustainable chemistry, the global chemical community began to rethink, revitalize and apply Green Chemistry principles in the teaching and research activities in research institutions and industries. At the turn of the century the number of publications related to Green Chemistry appeared were only in hundreds, but now they are in several thousands in various journals including a few dedicated journals like Chemical Education and Green Chemistry. At the turn of century, Pike Research also predicted the emergence of Green Chemistry in terms of global economic explosion.

The scope of this presentation is to go through all 12 Green Chemistry principles in detail with some examples. Historical milestones on the Green Chemistry will also be discussed. At the later part of the talk some of the real-world examples from the sustainability point of view are presented to stimulate the audience.

The primary goal of this talk is to empower and create thought provoking ideas among the staff and faculty so they can formulate this emerging Green Chemistry into their teaching methods to benefit students, who adapt it in further advancement of their careers whether they become scientists, teachers, administrators, law makers or business owners.

Molecular Materials

Prof. Jayanty Subbalakshmi

BITS-Pilani, Hyderabad

Molecular materials appeared propitious candidates, for variety of technologies in this century. On the account of flexibility, low cost, and lightweight, molecular materials represent remarkable departure from the traditional routes of material fabrication. Furthermore, molecular materials emerged as one of the thrust areas of research, especially in chemistry during the later half of the last century. Miniaturization of materials opened up the possibility to realize a vast range of magnificent and advanced applications, wherein researchers developed molecular devices based on small/single molecules with a wide variety of optical, electrical, mechanical, and semiconducting possessions. This talk shall focus on the molecular materials based on small molecules (organic donor-π-acceptors), polymers and fabrication techniques like crystallization, mechanical grinding and thin film coating.

ABSTRACTS

AB:01

Amberlyst-15 catalyzed Povarov reaction of *N*-arylidene-1*H*-indazol-6-amines and indoles: A greener approach to the synthesis of *exo*-1,6,7,7a,12,12a-hexahydroindolo[3,2-*c*]pyrazolo[3,4-*f*]quinolines as potential sirtuin inhibitors

Sushmitha Bujji, Nuty Vijaya

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Amberlyst® 15(H) has been shown for the first time to be effective as a greener catalyst in promoting the Povarov reaction between an imine, derived from the aryl/heteroaryl aldehydes and 1*H*-indazol-6-amine, and indole/5-bromo-1*H*-indole. Representative candidates from the library of *exo*-1,6,7,7a,12,12a-hexahydroindolo[3,2-*c*]pyrazolo[3,4-*f*] [3,4-*f*] quinolines, thus synthesized, were tested for their sirtuin (Sir-2) inhibitory activity using a yeast based assay. Five of the eleven synthesized compounds in the library exhibited closer to or greater than 50% inhibition, two of the most effective of them showing >75% inhibition of Sirtuin activity. Interestingly, all of these five active compounds were derived from 5-bromoindole and bore a semblance to the known potent sirtuin inhibitor, EX-527.

AB:02

Rational Drug Designing Approach to Identify New Bruton's Tyrosine Kinase Inhibitors

Savita[1,2], Radhika Vangala[1], SreeKanth Sivan[3,4] and Gururaj Somadi[4]*

[1]Department of Chemistry, St. Francis College for Women, Begumpet, Hyderabad
[2]Department of Chemistry, BITS, Pilani, Hyderabad Campus.
[3]Department of Chemistry, University College for Women, OU, Koti, Hyderabad.
[4]Department of Chemistry, Nizam College, OU, Basheerbagh, Hyderabad.

Bruton's Tyrosine kinase (BTK) is a target for of B cell related diseaseand alsofor selective inhibition of B cells soit is a main cause for the Rheumatoid Arthritis. A series of 3-substituted pyrazolopyrimidine derivatives were selected as the inhibitors of Bruton's Tyrosine Kinase. Pharmacophore modeling, molecular docking, structure activity relationship like 3D and 2D QSAR, in silico ADME prediction studies were performed to design new chemical entity. This current study has been carried out to determine drug likeliness andthe binding mode of compounds. A five-point pharmacophore model ADDHR.92 was developed and generated using fifty-three (53) compounds and this pharmacophore model was used to derive a predictive atom-based 3D quantitative structure activity relationship analysis (3D QSAR). The model had an excellent correlation coefficient (R^2=0.962) statistically significant as shown by Fisher ratio (F=227.7). The model also exhibited good predictive power confirmed by the high value of cross validated correlation coefficient (Q^2 = 0.7324).Molecular docking studies were carried out to understand the mode of interaction of inhibitors with the target receptor. This study will help us give an insight into designing novel inhibitors of BTK and provide a set of guidelines for designing compounds with improved Bruton's Tyrosine Kinase inhibitorypotential.

Key words: *Bruton's Tyrosine kinase (BTK), Rheumatoid Arthritis, Pharmacophore, Molecular docking*

AB:03

Synthesis, X-ray diffraction and Computational studies of N'-[furan-2-ylmethylidene]acetohydrazide

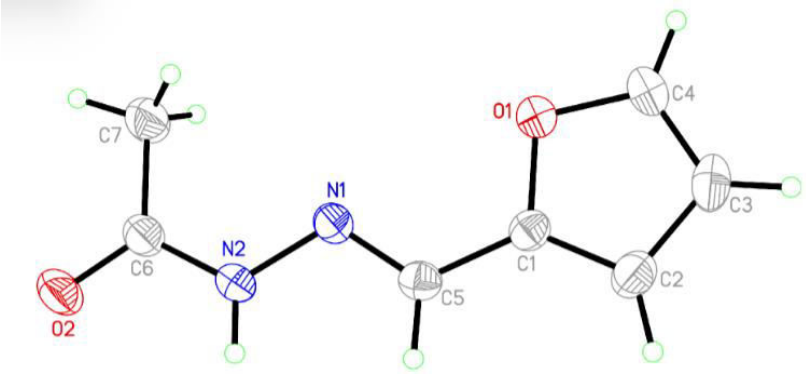
A.V. Aparna [a], Ch. Sarala Devi [b] *

[a.]Department of Chemistry, Nizam College, Osmania University, Basheerbagh, Hyderabad
[b.]Department of Chemistry, University College of Science, Osmania University, Hyderabad
* dr_saraladevich@yahoo.com

Hydrazones are important class of compounds in medicinal field. They are known to posses biological applications including anti-microbial, anti-convulsant, analgesic, anti-inflammatory and anti-tumorial activities. The acid hydrazides and their corresponding methyl hydrazides are of interest due to their remarkable biological activity. Studies revealed that the acetyl hydrazones can be used for protection against convulsions.

Many organic solids can exist in different physical forms. The present study focuses on the structural properties of a new polymorph of N'-[furan-2-ylmethylidene] acetohydrazide (NFMAH), by various spectro – analytical techniques viz; mass spectral, IR, ^{1}H – NMR, ^{13}C – NMR, DEPT and pH – metry. Polymorphism is often characterized as the ability of substance to exist as two or more crystalline phases that have different arrangements and/or conformations of the molecules in the crystal lattice. To understand the exact structure of new polymorph NFMAH, crystals were developed and were analyzed by the X-ray diffraction studies. Further, computational studies on NFMAH provided information regarding various physico-chemical properties. The frontier molecular orbitals, HOMO and LUMO computed for the neutral molecules and ionized species of the compounds indicated the presence of suitable orbitals on the possible coordination sites. As polymorphism is important in the development of pharmaceutical ingredients, it is planned to study the therapeutic activities of this compound.

Keywords: *N'-[furan-2-ylmethylidene] acetohydrazide (NFMAH), Spectroanalytical studies, XRD studies, Polymorphism, Computational studies*



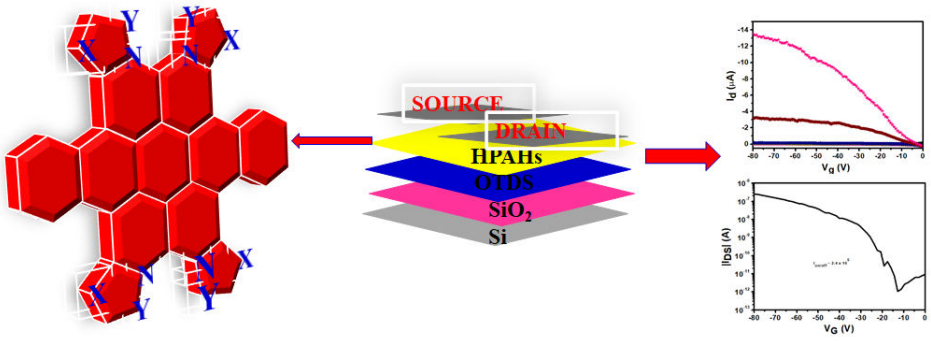
AB:04

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

Someshwar Pola

Department of Chemistry, Osmania University, Hyderabad, 500007

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



References

1. Y. -T. Tao, S. Pola, S. Kumar, M. M. Islam Synthesis and Characterization of Contorted Pentabenzo Fused Coronenes as Semiconducting materials, J. Org. Chem. 82 (2017) 8067-8071, https://doi.org/10.1021/acs.joc.7b01328.
2. S. Pola, C.-H.Kuo, W.-T. Peng, Md. M. Islam, I. Chao,Y.-T. Tao, Contorted Tetrabenzocoronene Derivatives for Single Crystal Field Effect Transistors: Correlation between Packing and Mobility, Chem. Mater. 24 (2012) 2566-2571, https://doi.org/10.1021/cm301190c.

AB:05

Molecular docking and 3D QSAR studies on DCN1 inhibitors

Ashwini K[1], Sudeepa K[2], Gururaj S[2] and Sree Kanth S[1]*

[1]Department of Chemistry, University College for Women, OU, Koti, Hyderabad.
[2]Department of Chemistry, Nizam College, OU, Basheerbagh, Hyderabad.

Cardiac fibrosis, one of the major global health problem, that is a common morphological feature of quite a lot of cardiovascular diseases. Defective in cullin neddylation protein 1 (DCN1) inhibitors can down regulate DCN1 activity leading to anti-cardiac fibroblast effect. Hence, a series of 2-(Benzylthio)pyrimidine derivatives reported as the inhibitors of Defective in cullin neddylation protein 1 (DCN1) were selected. Pharmacophore modeling, 3D QSAR and molecular docking were carried out to determine important pharmacophoric features and the binding mode of compounds. A five-point pharmacophore model AAHHR was developed and generated using fifty-three (54) compounds and this pharmacophore model was used to derive a predictive atom-based 3D quantitative structure activity relationship analysis (3D QSAR). The model showed good statistical reliability in terms of correlation coefficient (R^2=0.949), Fisher ratio (F=223.7). The model also exhibited good predictive power confirmed by the acceptable value of cross validated correlation coefficient (Q^2 = 0.662). Molecular docking studies were carried out to understand the mode of interaction of inhibitors with the target receptor. This study will help us give an insight into designing novel inhibitors of DCN1 and provide a set of guidelines for designing compounds with improved DCN1 inhibitory potential.

Key Words: *Cardiac fibrosis, Pharmacophore, Molecular docking, Defective in cullin neddylation protein 1*

Reference: *J. Med. Chem. 2022, 65, 163−190*

AB:06

Understanding oxidative phosphorylation inhibitor activity of benzene-1,4-disulfonamides by 3D QSAR studies.

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Bioenergetics and biomass production for cancer cells is depended on Glycolysis and oxidative phosphorylation (OXPHOS) processes. Inhibition of oxidative phosphorylation (OX-PHOS) is a potential therapeutic strategy for killing cancer cell that are dependent on aerobic metabolism. Recently, a series of benzene-1,4-disulfonamides derivatives were reported as Oxidative Phosphorylation Inhibitors. A Pharmacophore modeling and 3D QSAR analysis was to carried out to determine required pharmacophoric features for inhibitory activity. A five-point pharmacophore model AAAHH was developed and generated using fifty-three (54) compounds and this pharmacophore model was used to derive a predictive atom-based 3D quantitative structure activity relationship (3D QSAR) analysis. The model had an good correlation coefficient (R^2=0.977) statistically significant as shown by Fisher ratio (F=538.5). The model also exhibited good predictive power confirmed by the acceptable value of cross validated correlation coefficient (Q^2 = 0.652). This study will help us give an insight into designing novel molecules that can have inhibitory activity against oxidative phosphorylation

Key Words: *Oxidative phosphorylation, Pharmacophore, Molecular docking, cancer*

Reference: *J. Med. Chem. 2022, 65, 343−368*

AB:07

Understanding Pharmacophore Features of Aromatase Inhibitors to Identify Drug Like Molecules for Breast Cancer Treatments

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Breast cancer is the most common cancer among women worldwide. Most breast cancers in postmenopausal women are estrogen receptor positive (ER+). The proteinAromatase is responsible for the conversion of androgen to estrogen, which is the last and ratelimiting step in estrogen biosynthesis in peripheral tissues. Therefore, inhibition of aromatase is a promising method of developing new drugs for treating Breast cancer. Pharmacophore modelling, molecular docking, structure activity relationship like 3D QSAR, in silico ADME prediction studies were performed to design new chemical entity. The study has been carried out to determine the binding mode and drug likeliness of compounds. A three-point pharmacophore model ARR.10 was developed and generated using forty-three (43) compounds and this pharmacophore model was used to derive a predictive atom-based 3D quantitative structure activity relationship analysis (3D QSAR). The model showedagood correlation coefficient (R^2=0.8984), statisticalsignificancewas validated by external cross validated correlation coefficient (Q2 = 0.7069), which exhibits good predictive power. The information obtained from this study provide an insight for designing novel Aromatase inhibitors and provide a set of guidelines for designing compounds with improved Aromatase inhibitory potential.

Key Words: *Breast Cancer, Aromatase Inhibitor, Pharmacophore, Molecular Docking, QSAR*

AB:08

Synthesis and Biological Evaluation of Novel Oxa-Carbocycle Annulated Flavones

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Flavonoids are the prominent polyphenolic group of secondary metabolites found through the plant kingdom[1]. These compounds naturally occur in fruits, vegetables, seeds, nuts, flowers and play significant role in many biological processes. Flavonoids exhibit diverse type of properties that are useful for human health by interacting with a wide variety of cellular targets involved in cell signatory pathway in the body. Several therapeutically interesting biological, pharmaceutical activities of certain flavones have been reported including anti-cancer, anti-HIV, anti-oxidant, antimicrobial, ant arthritic, DNA cleaving, antianginous, ant hepatotoxic, anti-inflammatory, anti-mutagenic activities [2-3].

Here we describe a diversity oriented approach for the synthesis of skeletally different oxa-carbocyclic annulated molecular frame works like Oxepine-, Oxocin-, Oxepinone- annulated flavones (from more readily available starting materials) through the application of combined Claisen rearrangement and ring closing metathesis. The structures of all the synthesized compounds established by FT-IR, ^{1}H NMR, ^{13}C NMR, Mass spectral analysis and evaluated for their antioxidant and ant mycobacterialactivities

Keywords: *Hydroxyflavone, Claisen rearrangement, Ring closing metathesis, Grubbs' 1 and 2nd catalysts*

References

1. (a) J. B. Harborne, H. Baxter, *The Handbook of Natural Flavonoids*;, **1999**, 2, 8, 79. (b)S. A. Aherne, N. M. O'Brien, *Nutrition* **2002**, *18*, 75.
2. D. C. Rowley, M. S. T. Hansen, D. Rhodes, C. A. Sotrier, H. Ni, J. A. McCammon, F. D. Bushmanb, W. Fenicala, *Bioorg. Med. Chem.* **2002**, *10*, 3619-3625.
3. H. X. Xu, M. Wan, H. Dong, P. P. H. But, L.Y. Foo, *Biol. Pharm. Bull.* **2000**, *23*, 1072-1076;

AB:09

Conversion of Decalin over SBA-AC supported Pt catalysts

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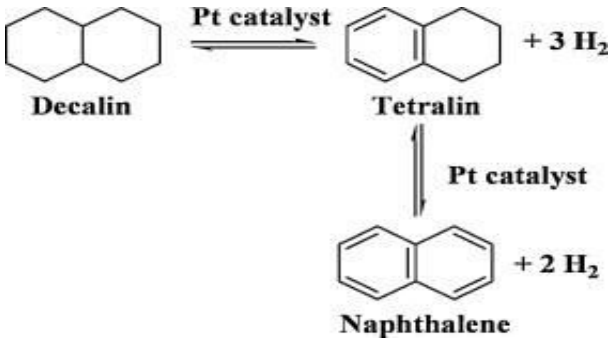
SBA-AC with a BET surface area of 530 m^2/g were used as the support to prepare the Pt catalysts investigated for decalin dehydrogenation to produce clean hydrogen and naphthalene over fixed bed reactor. About 136 x 10^{-6} molecules of hydrogen/ Pt molecule per sec with 75 % decalin conversion is endothermic were observed at 593 K.Organic hydride (decalin) as hydrogen storage media is an efficient source for fuel cells. Decalin is generally comprised of a mixture of*trans* and *cis* isomers, which have boiling points of 187°C and 196°C, respectively. Naphthalene has a boiling point of 218°C and is a solid at room temperature. *Cis*-Decalin shows higher conversion rate than*trans*-decalin, suggesting that the flexible geometry of *cis*-Decalin and it makes easier to be adsorbed on the catalyst surface. The potential yield of five moles of molecular hydrogen for each mole of decalin makes it a very attractive hydrogen donor compound for use in reactions which would otherwise require free molecular hydrogen. The synthesized catalysts were characterized by several techniques such as XRD, N_2-physisorption, H_2 -TPR, H_2 -chemisorption studies and physic-chemical properties.



Keywords: *Hydrogen Evaluation, Decalin, Dehydrogenation, Platinum catalysts.*

AB:10

Kinetics and Mechanism of Protection of Adenosine-5′-Monophosphate from Sulphate Radical Anion by Caffeic Acid under Anoxic Conditions

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The oxidation of adenosine-5′-monophosphate by sulphate radical anion ($SO_4^{\bullet-}$) has been followed by measuring the absorbance of adenosine-5′-monophosphate at 259nm spectrophoto metrically. The rates and the quantum yields (ϕ) of oxidation of adenosine-5′-monophosphate by $SO_4^{\bullet-}$ have been determined in the presence of different concentrations of caffeic acid. Increase in [caffeic acid] was found to decrease the rate of oxidation of adenosine-5′-monophosphate suggesting that caffeic acid acts as an scavenger of $SO_4^{\bullet-}$ and protects adenosine-5′-monophosphate from it. $SO_4^{\bullet-}$ competes for adenosine-5′-monophosphate as well as for caffeic acid. From the results of experimentally determined quantum yields (ϕ_{exptl}) of oxidation of adenosine-5′-monophosphate in presence of different concentrations of caffeic acid and the quantum yields calculated (ϕ_{cal}), $\phi_{cal} = \phi^0_{exp\,tl} \times p$, p is the probability of $SO_4^{\bullet-}$ reacting with adenosine-5′-monophosphate in presence of caffeic acid and ϕ^0_{exptl} is the quantum yield of oxidation of adenosine-5′-monophosphate in the absence of caffeic acid, assuming that caffeic acid is acting only as a scavenger of $SO_4^{\bullet-}$, show thatϕ_{cal} values are similar to ϕ_{exptl} values. This observation indicates that role of caffeic acid is restricted only to scavenge $SO_4^{\bullet-}$ and caffeic acid could not be able to repair adenosine-5′-monophosphate radicals produced on reaction with $SO_4^{\bullet-}$. These observations suggest that the adenosine-5′-monophosphate radicals are totally reducing in nature, unlike transient radicals produced in case of uracil, thymine, thymidine, adenine and adenosine reaction with $SO_4^{\bullet-}$. The oxidation of D- Ribose by $SO_4^{\bullet-}$ has been followed by measuring the absorbance of D - Ribose at 480nm spectrophotometrically using phenol sulphuric acid method. The oxidation of D- Ribose by $SO_4^{\bullet-}$ is one order of magnitude lower than the rate of oxidation of adenosine-5′-monophosphate. Independent estimation of the sugar moiety in adenosine-5′-monophosphate at different times also shows that sugar moiety is not oxidized considerably. Further rate of oxidation of adenine under similar condition is closer to adenosine-5′-monophosphate . These results therefore indicate that the base moiety might be the site of attack by $SO_4^{\bullet-}$ in adenosine-5′-monophosphate.

Keywords: *Oxidation of caffeic acid, protection of adenosine-5′-monophosphate by caffeic acid, Oxidation by sulphate radical anion.*

AB:11

Interaction of Vanadium metal complexes with PTP-1B enzyme

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Increased incidence of type2 diabetic mellitus (T2D) and obesity has elevated the medical need for new agents to treat the disease states. Resistance to the hormone insulin and leptin are hallmarks of both T2D and obesity. Evidences from biochemical, genetic and Pharmacological studies strongly suggest that inhibition of PTP-1B enzyme could address both diabetes and obesity and thus making PTP-1B as an exciting target for drug development. Studies have also showed that the over expression of PTP-1B is involved in diabetic and obesity patients and therefore inhibition of PTP-1B may be an effective strategy in the treatment of these patients. Although many natural PTP-1B inhibitors showed promising clinical, potential, there is no clinically used PTP-1B inhibitor which is most likely due to relatively low activities or lack of selectivity. Search for more potent and selective PTP-1B inhibitors is still necessary. Few organo vanadium metal complexes are synthesized and characterized (chapter-3). In addition, we evaluated the PTP-1B inhibitory effects of these vanadium metal complexes theoretically (molecular modeling) and experimentally (enzyme kinetics), results and discussions are presented in this chapter.

Keywords: *Vanadium complexes, T2D, PTP-1B, Fluoremetry, Stern-Volmer constant*.

AB:12

Validated HS-GC Method for Estimation of Residual Solvents in Rifapentine API

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Residual solvents are undesirable components present in Active Pharmaceutical Ingredient (API), excipients or drug products. To meet the specific quality- based requirements, the presence of these solvents in the pharmaceutical products should be monitored to ensure its safety. A novel, accurate, sensitive and simple method has been described for the estimation of residual solvents- methanol and dichloromethane in Rifapentine API by Head Space Gas Chromatography(HS-GC) coupled with Flame Ionization Detector(FID) using dimethyl formamide as diluent and separation was achieved on a DB-624 column(30m × 0.53mm, 3.00µm). The method developed was validated as per International Conference for Harmonization (ICH) guidelines for the parameters like- repeatability, linearity, range, ruggedness, limit of detection(LOD), limit of quantification(LOQ), and recovery studies. The linearity range selected was 25-150ppm and the correlation coefficient(r^2) values for all the solvents was found to be >0.99; recovery studies values were in a range 95-110% and %RSD values were also found to be not more than 5 for the solvents. Excellent results have been observed for all the validated parameters with good peak resolution and lesser retention times.

Key words: *Rifapentine, Residual Solvents, Head Space Gas Chromatography, International Conference on Harmonization.*

AB:13

An efficient F^- removal from groundwater by Carbon Alumina Composites Materials

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Fluoride is a highly reactive element among the elements in periodic table thus in nature it does not exists in the form of fluorides in a number of minerals of which fluorspar, cryolite and fluorapatite are the most common. Inorganic fluorine compounds are being used in various industries like aluminium production, steel and glass fibre industries, production of phosphate fertilizers, bricks, tiles and ceramics etc. Untreated effluents from these industries containing fluoride will contaminate the ground water by anthropogenic activities. Ground water is getting contaminated by natural leaching process of the fluoride from rock-minerals and also by anthropogenic activities. In some areas fluoride, in the form of fluorosilicic acid, sodium hexafluorosilicate and sodium fluoride, is being added to municipal water for the strength of the bone and teeth. Though fluoride is an essential mineral nutrient to the mankind to prevent dental cavities and for healthy bones, excess intake of fluoride in to the body results in various health disorders like osteoporosis, arthritis, hip fracture, cancer, Alzheimer's, brain damage and Thyroid disorder etc. According to WHO in 1996 limitations fluoride concentration must be in the range of 1 – 1.5 ppm, majority of the human population depends on the ground water for their thirsty needs. Thus it has become an utmost important for the synthesis of an efficient material to remove fluoride from ground water. This article discloses the synthesis of an efficient defluoridation composite material using Carbon, Alumina (CACM) its characterization and defluridation activity. Defluoridation property of adsorbents carbon alumina composite materials CACM-5, CACM-15, CACM-25 and CACM-50 was compared with commercially available carbon and γ – alumina. N_2 adsorption studies on all theses adsorbents reveal that CACM-25 prepared in exhibits highest surface area than C, Al_2O_3 materials prepared by physical mixing method (figure -1). However, defluoridation activity can be correlated with CO_2 pulse chemisorptions activity (figure -2). This concludes that carbon alumina composite materials prepared by deposition precipitation method with appropriate weight percentage of carbon as 25 exhibited an excellent defluoridation activity.

AB:14

Various Environmental Segments

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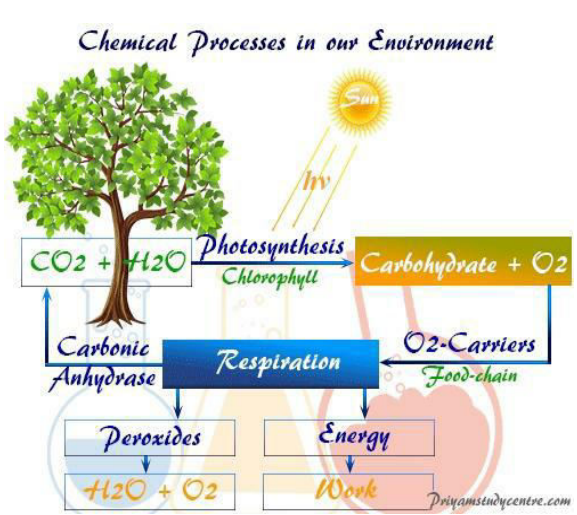
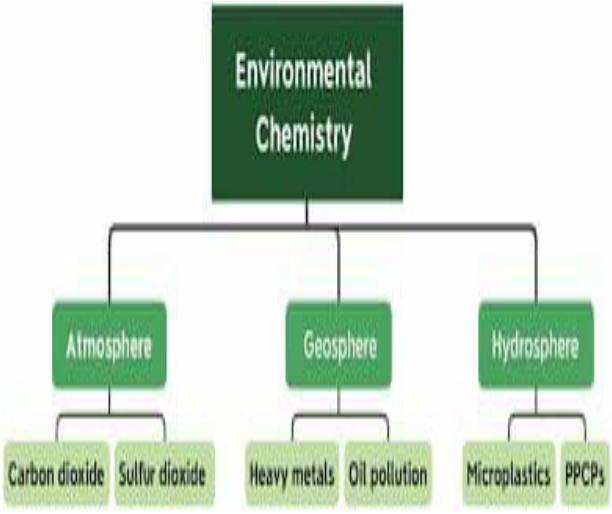
The study of chemical and biological events that occur in nature is known as environmental chemistry. It entails knowing how the unpolluted environment functions, as well as which naturally occurring chemicals are present, at what concentrations, and with what impacts. It would be hard to investigate precisely the effects that humans have on the environment through the release of chemical species without this. It is a multidisciplinary science that includes physics, life science, agriculture, material science, public health, sanitary engineering, and other fields in addition to chemistry. It is the study of the sources, reactions, transport, effects, and fate of chemical species in the air, water, and land, as well as the impact of human activities on various environmental segments, such as the atmosphere, hydrosphere, lithosphere, which consists of abiotic or physical environment, and biosphere, which is the fourth segment of the environment and consists of flora and fauna. The biome environment is made up of both abiotic and biotic components. The chemicals prevalent in the environment are both harmful and non-toxic in nature. Toxic chemicals released by industry into the air, water, and soil find their way into the human food chain through the environment. When these compounds enter the biological system, they disrupt natural biochemical processes, resulting in negative consequences. At the national level, there was a strong need for environmental education, both formal and non-formal. The goal of environmental education is to inform the public about the importance of environmental protection and conservation, as well as the necessity to limit human activities that result in the indiscriminate discharge of toxins into the environment.





Keywords: *Atmosphere, Hydrosphere, Lithosphere, Biosphere*

AB:15

Design, Synthesis, Characterization, Molecular modeling studies and evaluation of Cu(II),Pd(II) complexes with novel Schiff base ligand derived from 3- amino coumarin

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Coumarin belong to the family of lactones containing benzopyrone skeletal frame work that are isolated from plant as well as total synthesis in the laboratory .Furthermore the pharmacological and biochemical properties as well as therapeutic application of coumarins depend up on the pattern of substitution.

In view of this Coumarins have attracted intense interest in recent years because of their divers pharmacological properties .Hence Coumarins have been reported to posess among others anti convulsunts , anti inflammatory,antioxidents ,analygesic,anti coagulants,antivirul activities.

The novel Schiff base ligand (FYMAC) synthesized by the condensation of Furfuraldehyde and 3- amino coumarin .The nature bonding and geometry of the transition metal complexes as well as a ligand have been deduced from elemental analysis Mass,NMR,IR,ESR and thermal analysis .The complexes are found to have ML4 based on elemental,conductance and spectral studies

Octahedral (Cu) ,Square planar(Pd) geometry was assigned for these complexes.The geometry and stability can also be explained with computational studies. The ligand as a tetra dentate and co ordinate through N-atom of azo methane group O-atom of keto group of 3-amino coumarin.

Keywords; *Schiffbase,3-aminocoumarin,Metal complexes.*

AB:16

Microwave assisted synthesis of flavonoid based 1,2,3-triazole, isoxazoles towards evaluation of their antibacterial, antioxidant and anticancer activities

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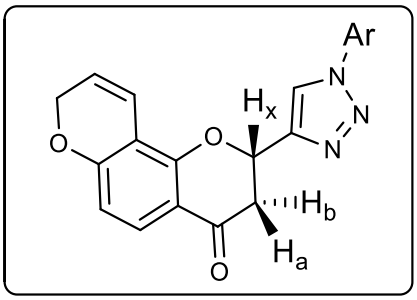
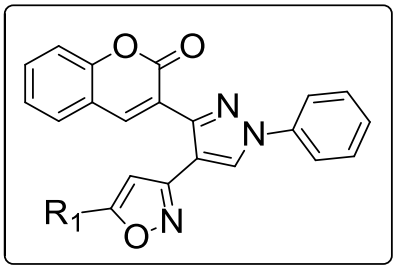
A new flavonoid based 1,2,3-triazole and isoxazoles in a simple and easily accessible microwave irradiation and conventional heating methods however, compounds synthesized by microwave irradiation gave good yields. Structures of all the synthesized compounds confirmed with IR, ^{1}H, ^{13}C and Mass spectral analysis. All the analogues subjected to *in vitro* for antibacterial activities, antioxidant activities and anticancer activities**.** Compounds **3c**, **6e**, **6f** and **6h** showed maximum *antibacterial* activity carried out with gram positive pathogens *Bacillus subtilis*, *Staphylococcus aureus* and gram negative species *Escherichia coli, Pseudomonas aeruginosa* with Streptomycin as a standard drug and *antioxidant* radical scavenging activity with Ascorbic acid as a standard drug, Furthermore, *anticancer* activity with MCF-7 and HeLa cell lines carried out with Doxorubicin standard drug and compounds **3c** and **6e** showed good results.





Keywords: 2-*H Chromene, 1,2,3-Triazole carbaldehyde, Chromenone, Antibacterial activity, Antioxidant activity and Anticancer activities etc.*

AB:17

Synthesis and Characterization of Insulin Mimetic Vanadyl Complexes and their Binding Studies with Bovine Serum Albumin

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over a century, vanadium salts (vanadylsulphate, sodium metavanadate, ammonium orthovanadate) have been shown to have insulin-like effects in improving the symptoms of Type II Diabetes Mellitus.The discovery by Lyonnet and Martin in 1899 which reported diabetic patients when treated with vanadate (VO4 3-) excreted less glucose in their urine was the first paper which gave an idea that vanadium salts can be used as metallotherapeutic agents. Later in 1985, Heyliger et al. reported the in vivo insulin mimetic activity of oral vanadate. Further studies confirmed that vanadium compounds are effective for lowering plasma glucose levels in diabetic subjects. Recently, it has been proved that the complexes of vanadium with organic ligands seemed to be less toxic than inorganic vanadium salts. A comparative study between VOSO4 and VO (AA)2 (Vanadyl (IV) bis(acetyalacetonate)) has shown that organic vanadyl complex performed much better than inorganic salt because of its greater hydrolytic and redox stability.It was concluded that VO (AA)2 was a more potent stimulator in lipid metabolism compared to VOSO4.In the current study,vanadium complexes of substituted β-diketones were selected based on the results of vanadium (IV) bis (acetylacetonate).Different methods were attempted to develop binary (1:2) vanadium complexes.All the complexes are characterized by UV-Vis, IR, Mass spectral studies, conductivity measurements. Potentiometric studies were conducted to examine the stability of complexes at different pH values. Further, the interactions of vanadium complexes with Bovine serum albumin (BSA) were done by dialysis technique. Consequently, binding (absorption) properties were studied using UV-Vis spectroscopy.

AB:18

Modeling Inhibitory Activity of Substituted Benzimidazoles

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In this work antibacterial MIC activity of various substituted benzimidazole against Gram positive bacteria bacillus cares have been modelled. The topological parameters viz. Geary autocorrelation lag/weighted by atomic Sanderson electronegativites and atomic polarizabilities have been found to be most suitable descriptors for modelling the antibacterial activity of present set of compounds. . The best three-parametric model gave value of R2 = 0.826. This model was validated by cross validated parameters. The electronegativity and polarizability parameters have been found to be useful in modeling the antibacterial activity of present set of compounds.

log I/CMIC = 2.5033 (+ 0.5278) GATS1e-1.4560 (+ 0.7247) GATS1p-
17.0471(+ 2.6512) GATS4p+21.5058

N=16, Se=0.3209, R2=0.826, R2Adj = 0.7825, F-ratio= 18.992, Q=2.832

We have also estimated log 1/CMIC using the above model the values obtained are in good agreement with experimental values. To find out the quality of model a graph between observed and estimated 1/CMIC values has been plotted which confirm that the proposed model is most suitable for modeling antibacterial activity of present set of compounds.

Few higher parametric models were also attempted but the variation in R2 & R2A did not support to use those models.

AB:19

Smart Agroecosystems using Nanosensors

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Agroecosystems are a source of food for mankind. Major challenges faced by agroecosystems include perpetual fluctuating climatic conditions, unceasingly demographic strain, the persistence of lethal heavy metals, and high utilization of resources. To fulfill the food requirements of an ever-growing population, the existing agricultural practices make use of sophisticated machinery, and agrochemicals which have led to an increased level of pollution and deterioration of soil health, thereby affecting human health.

Monitoring of agroecosystems is generally carried out by various methods which include High-performance liquid chromatography, mass spectroscopy, gas chromatography, etc. But these are high cost, time-consuming, and require skilled personnel. Hence there is an emergent need for quick and economically viable monitoring methods. Nanotechnology has offered rapid development of Nanosensors and biosensors for the detection of contaminants, biological components, and particular molecules. The present paper focuses on various biosensors and nanosensors employed in agroecosystem monitoring and the factors affecting their implementation.

Keywords: *Agroecosystems, challenges, Nanosensors, Biosensors, Factors affecting*.

AB:20

RP-HPLC Method Development and Validation of Levoflaxacin in Bulk Drug and Pharmaceutical Dosage Form

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A simple specific and accurate RP-HPLC method has been developed and validated of Levoflaxacin in bulk drug and pharmaceutical dosage forms. The chromatographic conditions were viably created for the unit of Levoflaxacin by using Inertial - ODS C18(250 x 4.6 mm,5µ), stream is 1.0 to 1.2 ml/min, convenient stage extent was Methanol: Water (75:25v/v),recognizable proof wave length was 250nm. Acetonitrile was used in this experiment. The results of the tablet analysis were validated with respect to accuracy (recovery), linearity, limit of detection (LOD) and Limit of quantification (LOQ) were found to be satisfactory.

KEY WORDS: *Levoflaxacin, RP-HPLC, Acetonitrile, Accuracy, linearity, limit of detection (LOD) and Limit of quantification (LOQ)*

AB:21

Development and Validation of a High-Performance Liquid Chromatography Method for Capmatinib Analysis

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Another methodology was set up for synchronous estimation of a Capmatinib by RP-HPLC system. The chromatographic conditions were viably created for the unit of Capmatinib by using Inertsil - ODS C18(250 x 4.6 mm, 5µ), stream is 1.0 ml/min, convenient stage extent was Methanol: Water (90:10), recognizable proof wave length was 255nm.Acetonitrile was used in this experiment.The results of the tablet analysis were validated with respect to accuracy (recovery), linearity, limit of detection(LOD) and Limit of quantitation (LOQ) were found to be satisfactory.

Key words: *Capmatinib, RP-HPLC, Acetonitrile, Acuracy,linearity, limit of detection (LOD) and Limit of quantification(LOQ)*

AB:22

Study of Photo catalytical, antimicrobial activity, dielectric and ac impedance properties of Zn doped Mg nanoferrites synthesized From Citrate Gel Auto Combustion method

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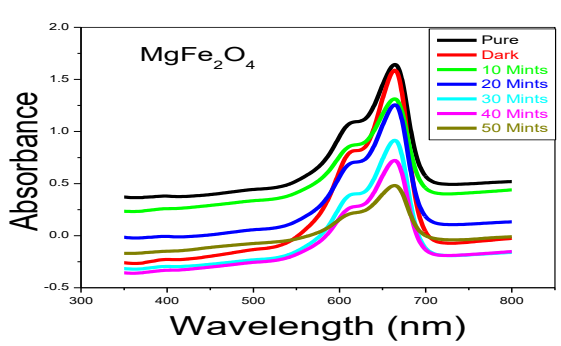
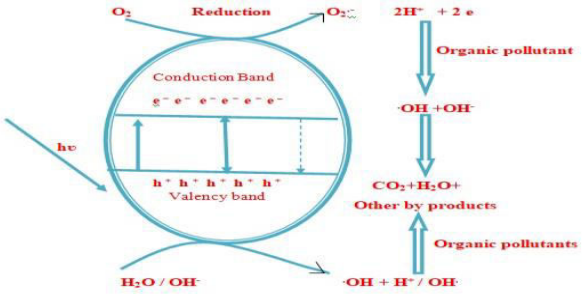
Mg-Zn nano ferrites with composition $Mg_{(1-x)}Zn_xFe_2O_4$ where ($0 \leq x \leq 1$) were synthesized through citrate gel auto combustion method with step wise variation 0.2 mol%. XRD revealed the formation of nano-sized particles with cubic spinel structure, the crystalline size decreased with increase in the Zn concentration, which ranged from 25 to 35 nm. SEM micrographs revealed inhomogeneous grains with agglomerates. UV- Visible spectroscopy confirmed the direct allowed transitions and optical band gap increased from 2.61ev to 2.71 with the addition of dopant Zn. The PL spectroscopy revealed that the broad near band edge excitation in visible range 350 to 450 nm wavelength region. Antibacterial efficiency of the nano ferrites enhanced with the antibacterial dopant element Zn against gram positive Bacillus subtilis (MTCC 121) and gram negative Escherichia coli (MTCC 1687) strains. Organic dyes such as methylene blue and acid red were used to do photocatalytical degradation process and significant rate of degradation was found. Frequency dependent AC conductivity (σ_{ac}) of the nano ferrites increased as a function of temperature and dopant Zn content. Dielectric parameters such as dielectric constant, dielectric loss (tan δ) were decreased with applied frequency. The results of dielectric studies reveals that the dielectric dispersion because of the hopping mechanism of electrons takes place in between Fe^{2+} and Fe^{3+} ions.





Key Words: *Citrate gel auto combustion method, XRD, photocatalytic activity, Dielectric studies.*

AB:23

Quantitative structure activity relationship and docking study of some influenza neuraminidase inhibitors.

Abha Shrivastava, Dr. Vijay k Agrawal.

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Neuraminidase inhibitors are class of drugs which block the Neuraminidase enzyme. There are two major classes of antivirals available for the treatment and prevention of influenza, the M2 inhibitors and the Neuraminidase inhibitors.
The Neuraminidase inhibitors zanamivir, laninamivir, oseltamivir and peramivir have been commercialized and have been demonstrated to be potent influenza viral Neuraminidase inhibitors against most influenza strains .

In this paper we have taken 55 compounds which are derivatives of 2-thiazolyl-hydrazone reported by Man-Ying Cuiet.al they are divided into two sets. A group of 41 compound as training set and 14 compound as test set. We modelled the PIC50 Activity using ATSC8s, P_VSA_MR_6 and RDF055p Parameters. The excellent value of R2 = 0.9555 shows that following model is best suitable.

We also performed docking study using various descriptors. With the help of Docking we proposed drug protein correlation.

Keywords: *QSAR studies, Docking, Neuraminidase inhibitors, Topological indices.*

AB:24

Experimental and theoretical investigation of Schiff base complexes derived from 3-{1-[(1H-Benzimidazol-2-yl)-hydrazono]-ethyl}-4-hydroxy-5-methyl-pyran-2-one

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A new Schiff base 3-{1-[(1H-Benzimidazol-2-yl)-hydrazono]-ethyl}-4-hydroxy-5-methyl-pyran-2-one(BHEMP) has been synthesized and metal complexes of the Schiff base were prepared from chloride salts of Co(II), Ni(II), Cu(II) and Zn(II) in ethanol medium. The Schiff base ligand and metal complexes were characterized by employing thermo gravimetric and various spectro-analytical techniques. The ligand behaves as neutral tridentate with three donor (NNO), and coordinates to metal atom in all the complexes by two azomethine nitrogens (ring and free) and oxygen atom of pyran group. A detailed analysis is done theoretically using DFT method with B3LYP/6-31G (d,p)functional for ligand and complexes. Based on experimental and theoretical data, structures are proposed for the present class of complexes. The antibacterial activity of the synthesized complexes is satisfactory.

AB:25

Geometry Optimization and Non-isothermal Kinetic Parameters Evaluationof Co, Ni and Zn Binary Complexes of Schiff Base derived from 3-Hydrazino-1,4-Benzoxazine-2-one and 4-hydroxy-3-methoxy benzaldehyde

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Thermogravimetric analysis-TGA is a technique used to evaluate the stability of complexes from thermogram. Thermal stabilities of Co, Ni and Zn binary metal complexes of Schiff Base derived from 3-hydrazino-1,4-benzoxazine-2-oneand 4-hydroxy-3-methoxy benzaldehyde were evaluated by TGA analysis.

The Kinetic parameters- (E_a)activation energy, (ΔH)enthalpy, (ΔS) entropy and (ΔG) free energy changes, were determined in the current study by the thermogravimetric data obtained.

The kinetic and thermodynamic parameters for the degradation of these binary metal complexes were calculated using Coats-Redfern (CR) integration method involvingthirteen kinetic models.

In this study, geometry optimization wasperformed and the stabilitiesof the metal complexes were also evaluated from the molecular orbital structures from which the quantum chemical parameters were calculated using HOMO and LUMO energies.

Keywords: *Activation energy, geometry optimization, quantum parameters, non-isothermal kinetic parameters, Coats-Redfern method.*

AB:26

Synthesis, Characterization And Antimicrobial Activities of Transition Metal Complexes Derived from Aminopyrimidine Schiff Bases

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A Schiff base ligand has been synthesized by the condensation of 2-amino-4,6-dimethylpyrimidine and 2-Hydroxybenzaldehyde. Metal complexes of the Schiff base were prepared by the reaction of the Schiff base and cobalt nitrate in ethanol solution. The complexes isolated, washed and dried. The Schiff base is pale yellow, while cobalt complexes is light yellow.The synthesized compounds have been characterized by FT-IR, ^{1}H-NMR and UV-Vis techniques for the ligands and FT-IR, UV-Vis, all reactions monitored by TLC, molar conductivity and magnetic susceptibility measurements for the corresponding complexes. General formula of complexes are $[Co(L_1)_2(H_2O)_2]$. The complexe is paramagnetic. The results of the molar conductivity measurements indicated that all complexes are non-electrolytes in (DMSO). An octahedral geometry for all the complexes of. The ligands are bidentate, (L_1) through phenolic (OH) and azomethine nitrogen.The ligand and its complexes were screened for their antifungal and antibacterial activity against *Aspergillus niger, Penicillium chrysogenum, Fusarium moneliforme, Aspergllus flavus* and *Escherichia coli, Salmonella typhi, Staphylococcus aureus, B. subtilis.* The result indicated that the complexes exhibited good antifungal and antibacterial activities.

Keywords:*Heterocyclic Schiff bases, 2-hydroxybenzaldehyde, 2-amino-4,6-dimethylpyrimidine, Antimicrobial Activity.*

References:

[1] D.T.Sakhare, Synthesis, characterization of some transition metal complexes of bidentate Schiff base and their antifungal and antimicrobial studies,Advances in Applied Science Research, 2015, 6(6):10-16.

[2] Kumar, N, Pratima, S, Aastha, P and Prasad, AVGS (2013). Synthesis and characterization of some new shiff bases. International Journal of Chemical and Pharmaceutical Sciences 23(2):231-236.

[3] Chigurupati S., (2015) Designing New Vanillin Schiff Bases and their Antibacterial Studies. Journal of Medical and Bioengineering, 4, 5, 363-366.

[4] Usharani, M, Akila, E, Ashokan, R and Rajavel, R (2013) Pharmacological Properties of Schiff Base Metal Complexes Derived From Subsituted Pyridine And Aromatic Amine – A Review, International Journal Of Pharmaceutical Science And Health Care, 3(5):2249 – 5738.

AB:27

Effect on the structural and optical properties of Cerium substitution Co-Mg mixednano ferrites by citrate gel auto combustion method

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From citrate gel auto combustion method Ce co doped Co-Mg mixed nano ferrites synthesized. The synthesized samples structural characterization has been done by XRD, SEM,EDAX, FTIR,UV-VIS. Spectroscopy. From x-ray diffraction studies, reveals that synthesized samples are in crystalline nature, as well as in nano meter region, which is 13.15nm to 23.13nm. Lattice parameter and X-ray density increases with increasing Ce Concentration on Co-Mg Mixed nano ferrites. Morphology of the synthesized samples was studied using scanning electron microscope (SEM). The elemental analysis of all the Cu-Zn-Ce nano ferrite samples with different compositions was analyzed by Energy Dispersive Spectrometer (EDS). FTIR spectroscopy used to find the functional group analysis of the materials. Optical absorption behavior of the synthesized samples carried out by UV visible spectral analysis. The observed results can be explained on the basis of composition and crystal size.

Keywords: *citrate-gel auto combustion method, X-ray diffraction, SEM, EDS, FTIR, UV visible spectra.*

AB:28

Photocatalytic studies of Cations (Ag^{+} and Sn^{2+}) Substituted $Na_2BaMg(PO_4)_2$

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We have synthesized visible light active silver/tin doped $Na_2BaMgP_2O_8$ (hereafter NBMP) photocatalysts via a solid-state/ion-exchange method. Powder X-ray diffraction (XRD), SEM-EDS, FT-IR, UV–visible diffuse reflectance spectra and X-ray Photo electron Spectroscopy measurements were employed to characterize all the samples. The substituted compositions adopted crystallizes in a hexagonal unit cell with the space group P63/m (176). The bandgap energy of the cations substituted samples were lower compared to that of parent NBMP. The photocatalytic activity of all the samples was studied against the degradation of methylene blue and methyl violet under visible light irradiation. Silver doped NBMP have exhibited higher activity compared to tin doped NBMP and parent material. The role of reactive intermediate species in the photocatalytic degradation of dyes was also studied using appropriate scavengers.

Keywords: *Powder X-ray diffraction, X-ray Photo electron Spectroscopy, Photocatalytic activity*

AB:29

Kinetics and Mechanistic Investigations in the Oxidation of Chloramphenicol by N-Bromosuccinimide

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In recent years, emerging organic contaminants are frequently detected in the environment and attract great attention due to their persistance and toxicity [1,2]. Contamination of pharmaceutical and personal care products (PPCPs) in surface waters and groundwater has been a potential threat to ecosystems and human health. Generally, PPCPs are difficult to be removed sufficiently by the conventional water treatment processes due to their complex polymer structure and antibacterial property. The presence of antibiotics in the aquatic environment negatively impacts the growth and reproduction of organisms [3].The extensive use of antibiotics in the treatment of bacterial infections has brought about serious contamination in aquatic environments including surface water and groundwater.As a result, the development of techniques that effectively remove antibiotics during drinking water treatment is a top priority.Chloramphenicol(2,2-dichloro-N-[(1R,2R)-2-hydroxy1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl]acetamide, CHP) commercially known as chloromycetin [4] is considered as a prototypical broad-spectrum antibiotic, alongside the tetracyclines, a chlorinated nitroaromatic antibiotic with excellent antibacterial properties. Kinetics and mechanistic studies in the oxidation of chloramphenicol has been studied using N-Bromosuccinimide(NBS) in alkaline medium in the presence of mercuric acetate. The reaction followed first order kinetics in [NBS], fractional order each in substrate and alkali. The reaction was studied at different temperatures and the corresponding activation parameters were evaluated. The oxidation product was identified as *p*-nitrobenzaldehyde. Based on the experimental observations a probable mechanism has been proposed and a suitable rate law has been derived which explains the above results.

References:

1. Q.Q. Zhang, G.G. Ying, C.G. Pan, Y.S. Liu, J.L. Zhao, *Environ. Sci. Technol.* 49 (2015) 6772.
2. B. Petrie, R. Barden, B. Kasprzyk-Hordern, *Water Res*. 72 (2015) 3.
3. J. Chen, G. G. Ying, W. J. Deng, *J. Agric. Food Chem*. 67(2019) 7569.
4. J. Ehrlich, D. Gottlieb, P. R. Burkholder, E. A. Lucia, T.G. Pridham, *J. Bacteriol*. 56(1948)467.

AB:30

Nutraceuticals vs Pharmaceuticals

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Gastrointestinal complaints, such as acid reflux, nausea and digestion problems are of prime importance as they continue to inflict about 44% population. Gastroesophageal reflux disease (GERD) is diagnosed when acid reflux occurs more than twice a week. GERD affects people of all ages, sometimes for unknown reasons, and this cannot always be prevented. Persistent exposure to stomach acid can damage the oesophagus leading to Oesophagitis, Strictures, Barrett's oesophagus etc. Many medications available are effective, but like any prescription drug like omeprazole often prescribed by medical practitioners, is not appropriate for all people with reflux disease and can cause side effects like absorbing nutrients, leading to malnutrition. Even among COVID-19 patients, these problems are noticed weeks after they have recovered from the infection. Gastrointestinal and digestive symptoms could also be caused by prolonged use of some of the medications used for COVID-19 treatment.

With the advent of Nutraceutical's an emerging science, there is growing interest in developing products with natural ingredients a plant origin to fight varied, ailments which prove to be effective, safest and economical. A proprietary food which is a powder made from seed species like pepper, carom seeds, cumin seeds, coriander seeds and dry ginger play an effective role in controlling acid reflux , flatulence, heartburn, blenching and any other digestive ailment not only in post, Covid -19 recovery patients but also any individual. This particular powder has 8 over hedonic scale for flavour, taste, aroma and ease of use. This is stable at room temperature for 6 months.

Our present study aims Comparison of the physico chemical properties of the proprietary mix with various drugs recommended for gastrointestinal problems.

Keywords: *Covid -19, acid reflux, malnutrition, Nutraceutical's, Proprietary*

AB:31

Increasing demand of Sustainable Cement to reduce pollution

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Cement is an essential component of construction material. The demand for cement production is increasing day by day. To meet the current infrastructural needs large amounts of cement has been manufactured annually all over the world. But Cement industries are facing many challenges globally as it is a heavy polluter. A major environmental issue from cement industry is carbon footprint. The emissions from carbon industry accounts for 6% of all man made carbon emissions and 4% of global warming. To build a sustainable future and to overcome the challenges faced by the cement industry there is an immediate need to adapt to alternative production methods. Novel cement formulations should be used. To produce sustainable cement, techniques like carbon capture and storage (CCS), cement replacement material, alternative fuels and energy efficient technologies have been identified in recent years. Supplementary cement materials like coal combustion fly ash, furnace slag, silica fume etc. are used in production of carbon negative cement. **Green cement** is such an innovation which reduces the carbon emissions to a greater extent when compared to ordinary Portland cement. It produced with the help of a carbon-negative manufacturing process. Recently Nanotechnology has also been used for sustainable cement production. Blended cements are a revolutionary product produced in an environmentally-friendly way and can help build a sustainable world.

Keywords: *carbon footprint, Green cement, Nanotechnology, Sustainability.*

AB:32

Study of critical micelle concentration and its thermodynamic properties of Sodium Dodecyl sulphate in the presence of additives.

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The critical micelle concentration (c.m.c) of Sodium Dodecyl Sulphate containing amono acids, sodium chloride and ethanol is determined using electrical conductivity method at various temperatures. Critical micelle concentrations have also been measured as a function of the concentration of alcohol added. It is suggested that alcohol addition leads to an increase in the micellization that depends on the alcohol chain length. Thermodynamic parameters were evaluated for micellar systems in presence of all the additives to further explain the results.

Key words : *Micelle, c.m.c. Conductivity, Alcohols*

AB:33

Structural Modification of Zolpidem Resulted Potent Anti-TB Activity In Imidazo[1,2-*a*]Pyridine/Pyrimidine-1,2,3-triazoles

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Ambien (zolpidem) is an imidazo[1,2-*a*]pyridine derivative, a commercial drug to treat insomnia which also possesses the antitubercular activity against *Mycobacterium tuberculosis* H37Rv. In this paper, we describe the synthesis of three diverse lead series of imidazo[1,2-*a*]pyridine/pyrimidine-1,2,3-triazoles (IPT) which are designed by specific structural modifications of the zolpidem. Most of the IPTs exhibited remarkable *in vitro* antitubercular activity with the MIC of 1.56 µg/mL, which is two-fold superior than the MIC of the zolpidem. Further, the synthesized IPTs displayed moderate inhibition activity against several bacterial and fungal strains as well, and also showedan acceptable safety profile as verified through *in vitro* cytotoxicity assessment against VERO cells. In addition, the potent IPTs exhibited promising binding interactions within the active site of InhA enzyme. An interesting correlation between the *in vitro* inhibition activity and the binding mode was observed that most of the potent molecules (MIC = 1.56 µg/mL) interact through H-bond with Tyr 158 residue of the target enzyme. These efforts toward the structural modification of the zolpidem could be helpful for further optimization of the IPT core to develop new anti-TB drugs.

Key words: *Imidazo[1,2-a]pyridine, Zolpidem, 1,2,3-triazole, Mycobacterium tuberculosis and molecular docking.*

References

1) Rattan, A.; Kalia, A.; Ahmad, N. *Emerging Infect. Dis.* 1998, 4 (2), 195−209.

2) Hegde, D.; Dodamani, S.; Kumbar, V. *Appl Organometal Chem*. 2017, 31, e3851.

AB:34

Synthesis and biological evaluation of D-Ring modified Amido derivatives of Podophyllotoxin as tubulin inhibiting agents

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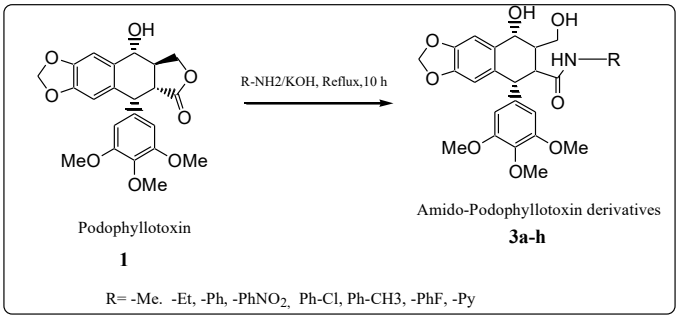
Podophyllotoxin, a well-known naturally occurring aryl tetralin lignan is extracted from the roots of *Podophyllum peltatum* and *Podophyllum hexandrum*. The medicinal properties of podophyllotoxin have been well-recognized for centuries.[1,2] However, the high toxicity and severe gastrointestinal side effects of podophyllotoxin have to be reduced before its use as a drug in cancer chemotherapy. Herein we report the synthesis of D-Ring modified Amido derivatives of Podophyllotoxin from the reaction between Podophyllotoxin and different amines. All the products were characterized by H^1-NMR, C^{13}-NMR, Mass, IR spectral studies. In our studies, it was found that these Podophyllotoxin derivatives were less cytotoxic and inhibit the assembly of tubulin into microtubules through interaction with the protein at the colchicine binding site eventually leading to apoptosis.



Scheme:- The synthesis of amido derivatives of Podophyllotoxin

References:

1. Ayres, D. C.; Loike, J. D. Lignans: Chemical, Biological and Clinical Properties; London: Cambridge University Press, **1990**.
2. Hartwell, J. L.; Scherecker, A. W. *J. Am. Chem. Soc*. **1951**, 73, 2909.
3. Loike, J. D.; Brewer, C. F.; Sternlicht, H.; Gensler, W. J.; Horwitz, S. B. *Cancer Res*. **1978**, 38, 2688.
4. Imbert, T. F.; *Biochimie* **1998**, 80, 207.

AB:35

Novel tryptanthrin hybrids bearing aminothiazolesas potential EGFR inhibitors: Design, synthesis, biological screening, molecular docking studies and ADME/T Predictions

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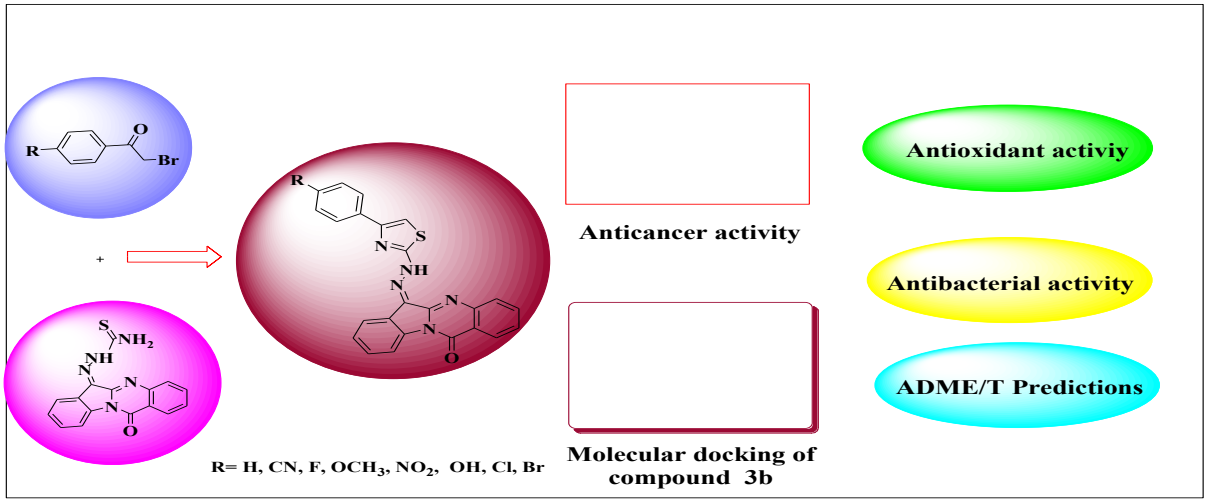
A variety of novel tryptanthrinaminothiazole analogues **3a-h** and **5a-h** possessing a biologically active thiazole moiety were synthesized by the reaction of tryptanthrinthio semicarbazones withdifferent α-bromo-4-substituted-acetophenones compounds. The structures of all the synthesized compounds were characterized by Mass, ^{1}H NMR, ^{13}C NMR, and elemental analysis. All the novel synthesized compounds were investigated for their *in-vitro* anticancer activity against three human cancer cell lines (MCF-7, A549, and HeLa) by taking cisplatin as a reference drug. The compounds **3b** and **3c** displayed excellent anticancer activities against the growth of three human cancer cell lines. EGFR targeting molecular docking investigation revealed that tryptanthrinaminothiazole analogues have better binding energies compared with EGFR inhibitors (Gefitinib, Erlotinib and Lapatinib). The molecular docking findings back up the experimental anticancer activity results very well. The compounds were also tested for their antibacterial and antioxidant activities. In silico ADMT predictions have performed that these tryptanthrinaminothiazole analogues have a good pharmacokinetic profile.



Keywords: *Tryptanthrinaminothiazole, Anticancer, Antibacterial, Antioxidant, Molecular docking, ADME/T Predictions*

AB:36

Synthesis and in Silico Molecular Docking Studies of Chalconebased 1,2,3-Triazoles

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A series of chalcone based 1,2,3-triazoles compounds are synthesized and screened for in vitro antimicrobial activities. Condensation of aldehydes and ketones results in the formation of chalcones. Acetylated chalcones and different aryl azides were cyclized to obtain chalcone based 1,2,3-triazoles through 1,3 dipolar cycloaddition (Click reaction). The products are confirmed with IR, ^{1}H and ^{13}C NMR and Mass spectral analysis and screened to evaluate their in vitro antimicrobial activities. Compounds**6j, 6c, 6g,6d** and **6k** showed excellent zone of inhibition compared to *Ampicillin* and *Bavistin* drugs. Molecular docking studies showed good H-bonding interaction with selected proteins.

AB:37

Validated UV- Spectrophotometric methods for the simultaneous estimation of Dextromethorphan and Guaifenesin

Dextromethorphan and Guaifenesin is a combination medicine used to treat cough and chest congestion caused by common cold or allergies. Using UV Spectrophotometric Methods, five simple, precise, and accurate approaches are devised and verified for the simultaneous assessment of Dextromethorphan (DEX) and Guaifenesin (GUA) in combined dosage form. The approach 1 employs solutions of simultaneous equations using, while the approach 2 called Q-ratio or isoabsorptive method based on measurement at iso-absorptive point as well as λmax of the other drug. The approach 3 is the Dual wavelength method, which was developed, evaluates the difference in the absorbance of mixtures at wavelengths where single drugs have the same absorbance and vice versa. Approach 4 is a mean-centered ratio method that relies on the production of calibration by dividing the spectra of one substance by the spectra of the other. Approach 5 is a derivative spectrum method that relies on the derivative spectrum's zero crossing points to create calibration for two medications in the presence of the second. To assess the accuracy and precision of all five approaches, six replication tests and recovery investigations utilising recognised synthetic blends are used. The calibrations are used to analyze two pharmaceuticals present in the tablet. The procedures have been validated in accordance with ICH recommendations.

KEYWORDS: *Dextromethorphan, Guaifenesin, Simultaneous equation, Q-Absorption, Derivative spectrum, Dual wavelength, Mean centered ratio method.*

AB:38

Computational Design, Synthesis and Activity Studies of coumarin based 1,2,3-Triazole derivatives as anticancer inhibitors

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A series of 1,2,3-triazoles compounds are synthesized and screened for *invitro* anticancer activity. Condensation of 7-hydroxy coumarin reacts with 4-hydroxybenzaldehyde in presence of glacial acetic acid, piperidine in ethanol affords (Z)-3-(4-hydroxybenzylidene)chromane-2,4-dione, further propargylation followed by reaction with different aryl azides cyclized and gave rise to 1,2,3-triazoles through 1,3 dipolar cycloaddition (Click reaction). The product confirmed based with IR, ^{1}H and ^{13}C NMR and Mass spectral analysis. The compounds screened to evaluate their in vitro anticancer activities. Molecular docking studies showed good H-bonding interaction with selected proteins.

AB:39

Sonogashira Reaction using Green methods

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Sonogashira reaction is powerful reaction. In which alkynes are formed by coupling terminal alkyne with Aryl and Vinyl halides in presences of a metal catalyst like Palladium or Copper which are commonly used. This reaction is used for the preparation of unsymmetrical alkynes. General reaction: -

$$R\text{-}X + Ph\text{-}\equiv\text{-}H \xrightarrow{Pd/Cu} R\text{-}\equiv\text{-}Ph$$

This reaction can be performed using green method by changing the solvent from Transition - Metal phosphine complex to water. By using water as solvent problems like intrinsic toxicity and air sensitivity of transition - metal complexes and the use of expensive phosphane ligands can be reduced.

Sonogashira Coupling under Transition - Metal free conditions involve ultra-low Pd concentration which cause contamination. Another Green method for performing this reaction involves usage of NaOH as base, Polyethylene Glycols (PEG) as phase transfer catalyst and water as solvent under microwave heating gave the coupled product in good yield .

Green Sonogashira Reaction: -

$$R - X + R\text{-}\equiv\text{-}H \xrightarrow[170\text{ degree centigrade},5\text{ minutes}]{NaOH,\ PEG,\ water,\ Microwave} R\text{-}\equiv\text{-}R$$

AB:40

Significance of imidazole ring in biological system

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Imidazole is a nitrogen containing 5 - membered Aromatic heterocyclic ring present in a number of natural products and synthetic molecules . The Imidazole ring has a peculiar structure with desirable electron rich characters which makes it beneficial for the imidazole derivatives to bind easily with a number of receptors and enzymes in the biological systems through weak interactions , thereby manifesting broad bioactivities . In humans , the imidazole core is present in components like Histidine, Histamine , Vitamin B12, Biotins, etc. Imidazole rings are also incorporated in many synthetic drug molecules like Cimetidine , Azomycin and Metronidazole . The role of imidazole - based compounds in clinical drugs for the treatment of various types of diseases with high therapeutic potential have made Imidazole significant for further research and development in medicinal chemistry . The drugs having the imidazole core have been found to exhibit Antibacterial , Anticancer , anti - tubercular , Antifungal , anti - analgesic , anti - HIV , Antioxidant , antidepressant , and antihypertensive activity. Some Substituted Imidazole derivatives like 2 - substituted - 4,5 - diphenyl - 1 H - Imidazoles have exhibited significant Anticonvulsant effects .

The 2 - iodo 4 - hydroxy methyl 1 - 1,5 diphenyl substituted 1 - H - imidazole derivatives were evaluated for Anti-cancer activity . The results when compared with standard drug inhibitors showed that the substituted imidazole derivatives exhibited significant inhibitory activity against Breast cancer . Imidazole and its derivatives are an interesting class of compounds that show a wide and diverse spectrum of biological activities. Moreover doing slight alterations in the substituent groups present on the imidazole ring have exhibited enhanced biological activity and less toxicity.

AB:41

Spectroscopic Analysis of interaction of Biomolecules(Proteins) with Nanoplanes

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Gold, silver, and copper are noble metal nanoparticles. Gold and silver nanoparticles have a wide range of biomedical applications in the fields of medical diagnosis, drug/gene delivery and bioimaging. Noble-metal-based nanoparticles, as one type of nanomaterial for biomedical applications have increased the chances of developing new diagnostic platforms for early disease and threat detection. Because of their unique characteristics such as size, shape, optical, electric and magnetic properties, silver nanoparticles (AgNPs) have gotten a lot of attention. The objective of this study is to dope nanoplanes with haemoglobin and determine their interactions at various time intervals using a titrimetric method as well as to dope nanoplanes with different proteins (lysozyme, trypsin, hemoglobin, and bovine serum albumin) before and after denaturation. The wavelength(nm) and absorbance of Dipole(D) and Quadrupole(Q) peaks of nanoplanes were determined. The results showed that no two nanoplanes doped with proteins have the same Q/D ratio and that the Q/D ratio gradually decreased. This discovery could be useful for detecting and analysing biomarker proteins in disease states. This paves the way for it to be used as a diagnostic tool. In the field of diagnosis, it is critical to detect biomarker proteins in disease conditions with high precision and in a short time frame. Our project develops a new platform for detecting biomarker proteins in a more precise and cost-effective manner using a small amount of protein.

Keywords: *Silver nanoparticles, nanoplanes, UV-VIS spectrophotometer*

AB:42

Bio-Inspired Green synthesis of Palladium Nanoparticles

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The Bio-inspired Green synthesis of palladium nanoparticles have attracted by its remarkable applications like anti-microbial, anti-inflammatory, anti-cancer and play a vital role in heterogeneous quantitative evaluation of catalytic activities such as reductions, oxidations, hydrogen storage and coupling reactions and environmental remediation purposes. In the present study, the Microwave assisted green biosynthesis of highly active palladium nanoparticles is carried out using non-toxic, renewable, naturally available plant resource Psidium guajava leaf extract as both reducing and stabilizing agent in aqueous media. Beside these the synthesis method shows many advantages such as shorter reaction times, use of environmentally benign solvent systems and mild reaction conditions.

The biosynthesized materials were characterized using UV-Visible spectrophotometer, XRD and DLS. The Palladium Nanoparticles formation was confirmed by the appearance of dark brown colour and absorption spectra in the UV-Visible region. The synthesized nanoparticles were found to be crystalline in nature. These nanoparticles were found to involve in the degradation of Methyl Violet and Methylene blue dye. Further, the palladium nanoparticles applications like Anti-Cancer activity, Anti-Microbial activity are to be evaluated.

Keywords: *Biosynthesis, Microwave, Palladium nanoparticles, X-ray Diffraction, Dynamic Light Scattering*.

AB:43

Ultrasound Assisted Synthesis and *invitro* Antibacterial Studies of Phenothiazine Derivatives

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A tricyclic heterocycle is an important moiety for a wide range of medicines. Phenothiazine, one of the most prevalent tricyclic compoundsconsisting of two benzene rings connected by sulphur and nitrogen atoms. Phenothiazine and its derivatives possess wide range of biological activities such as antimicrobial (1), antioxidant (2), anticancer (3) and other pharmacological activities. Phenothiazine containing chalcone derivatives**4a-h**were prepared via compound **3** with different substituted acetophenones in presence of alcoholic KOH under conventional and ultrasonic irradiation method. All the prepared derivatives were characterized using spectral techniques such as IR, NMR and Mass Spectral data. The compounds **4a-h** were tested for antibacterial activity against "Gram +ve" and "Gram -ve" bacterial strainby agar well diffusion method.Among those compounds **4d, 4g,** showed good activity against *S. aureus, P. aeruginosa, E. coli and K. pneumonia* and moderate activity against *B. cereus* while compounds **4g** exhibited significant activity against *B. cereus*. Compounds **4a, 4f** showed moderate activity against *S. aureus, P. aeruginosa, E. coli, K. pneumonia*.

References:

1. T.N.Bansode,J.V.Shelke, V.G.Dongre, Synthesis and antimicrobial activity of some new Nacyl substituted phenothiazines, Eur JMed Chem., **2009**, 44, 5094-5098.
2. C. Iuga, A. Camperob, A. Vivier-Bunge, Antioxidant vs. prooxidant action of phenothiazine in a biological environment in the presence of hydroxyl and hydroperoxyl radicals: a quantumchemistry study, RSC Adv., **2015**,5, 14678-14689.
3. G. Spengler, A.Csonka, J. Molnar, L. Amara, The Anticancer Activity of the Old Neuroleptic Phenothiazine-type Drug Thioridazine, Anticancer Res, **2016**, 36,5701-5706.

AB:44

Identification and optimization of promising human PTPM protein inhibitors against type 2 diabetes

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Protein tyrosine phosphatase mitochondrial (PTPM) moderatesbiosynthetic pathway of cardiolipin.An aberrant cardiolipin metabolism linked to numerous diseases andPTPM protein is considered as challenging drug target for type 2 diabetes. The lack of experimental evidence published yet about the 3D structure of PTPM proteinin protein databank paved the path for structure-based approach.The 3D structural model of PTPM proteinis build and refined through energy minimization in VMD-NAMD interface. Active site of PTPM protein is identified by SiteMap module (Schrodinger suite) and corroborated with literature reports.GLIDE molecular docking protocol is employed to identify novel chemical entities, which are prioritized based on their glide score and glide energy. Further the final molecules are rescored by calculating the binding free energy using Prime-MM/GBSA parameter. The identified novel leads are optimized andare further evaluated for their drug likeness by calculating the ADME properties. The outcome of the present study is accomplished for the development of novel chemical entities as potential inhibitors of human PTPM protein against type 2 diabetes.

Keywords: PTPM protein, cardiolipin pathway, type 2 diabetes, homology modelling, NAMD, Prime MM/GBS.

AB:45

Effect of soil pH on germination and growth of *Triticum aestivum* and *Zea mays*

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Various environmental stresses viz. extreme temperatures, problem soils including soil salinity, drought and flood have affected the production and cultivation of agricultural crops. Among these, problem soil (acidic, alkaline, sodic, and saline) is one of the most devastating environmental stresses, which causes major reductions in cultivated land area, crop productivity and quality caused by variable concentration of ions in the soil. Soil reaction (pH), in particular, is an important variable, perhaps due to its influence on many other soil properties and processes affecting plant growth. Many plant characteristics (i.e., traits) such as height, lateral spread, grains yield, biomass, flower size and number, pollen production, etc., are influenced by the pH of the soil. In this study, we investigated the effects of soil pH on the germination and growth (shoot and root height, yield, dry weight, etc.) of *Triticum aestivum* (bread wheat) and *Zea mays* (corn). Highly acidic soil (pH 4.0) was collected from a site (hotspot) in Sonipat district of Haryana. Simultaneously, problem soils, both acidic and alkaline soils were prepared by fortifying garden soil (pH 7.0) with weak acidic and basic solutions using aluminium sulphate and calcium hydroxide, respectively. Experiments were conducted with replicates, to counter experimental errors. A set of control pots having seeds of wheat and maize grown in garden soil was also set up.

Keywords: *Soil, pH, problem soil, Triticum aestivum, Zea mays*

AB:46

Charge Transfer Complex of 3,4-Ethylenedioxyaniline and DDQ: Synthesis, Spectral, Thermodynamic, Antimicrobial and DFT Studies

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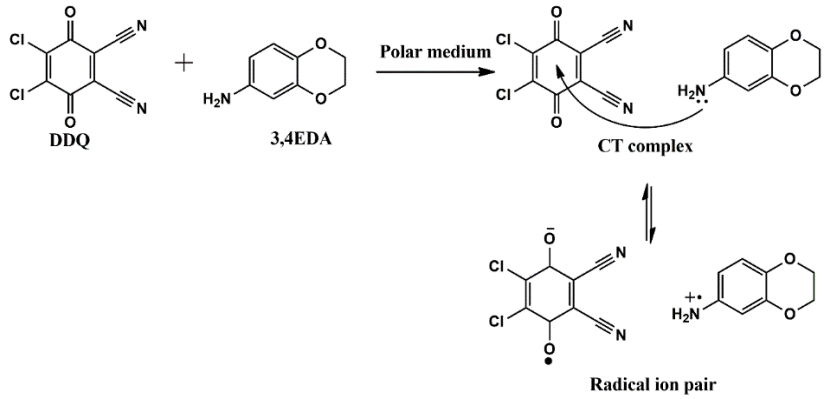
The charge transfer (CT) complex of the donor, 3,4–ethylenedioxyaniline(3,4EDA) with the π-acceptor 2,3-dichloro-5,6-dicyano-p-benzoquinone (DDQ) in acetonitrile medium has been studied spectrophotometrically at different temperatures. The molecular composition of the complex was studied by applying Job's continuous variation and spectrophotometric titration method. The 3,4EDA–DDQ CT complex have been prepared and characterised in solid and solution state by UV-Visible absorption, FT-IR, and ^{1}H-NMR spectral studies. Benesi–Hildebrand equation has been applied to calculate the formation constant, K_{CT} and molecular extinction coefficient, ε; thermodynamic and spectroscopic physical descriptors of the CT complex were investigated. The standard enthalpy (ΔH°) and standard entropy (ΔS°) of CT complex formation have been estimated by using van't Hoff equation. The signs of ΔH°, ΔS° and ΔG° reveal the CT complex formation process is stable, exothermic and spontaneous process.



The 3,4EDA-DDQ charge transfer complex was tested for pharmacology, including antimicrobial activity against a variety of bacterial and fungal cultures. Similar to standard drugs Tetracycline and Nystatin. The experimental studies were complemented by quantum chemical calculations at DFT (B3LYP/6-31G++ (d, p)) level of theory using Gaussian 09w software. It includes bond lengths, bond angles, Mulliken electron charge on atoms, molecular electrostatic potential maps and molecular orbital surfaces which are helpful in assigning the CT route. A good consistency was found between experimental and theoretical results.

Keywords: *Charge transfer complex, 3,4–ethylenedioxyaniline, Thermodynamic parameters, Antimicrobial, and DFT calculations*

AB:47

Preparation of biodegradable plastic composites from fruit wastes.

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Organic food wastes have been considered to be a barrier in sustainable development,as their decomposition leads to a tremendous increase in greenhouse gases and creates environmental problems. Similarly, when petroleum-based plastics are used in surplus amounts beyond control, it becomes amajor cause for environmental pollution. In order to overcome these issues and to minimise the plastic and food waste- based problems, biodegradable composites are being prepared as a substitute to these products. Bioplastics are defined as the plastics which are derived from natural resources like fruit waste, biomass, corn-starch, sugarcane and food waste. The bioplastics such as polyhydroxyalkonoates (PHAs) or polyhydroxybutyrates (PHBs) has the ability to replace a number of traditional plastics, which are made up of petrochemicals and serves as potential alternate to the conventional plastic material. These are partially or entirely biodegradable and are relatively less harmful to the environment.

The primary objective of this study is to produce biocomposites from fruit wastes and peels using simple laboratory techniques and to characterize them for various physical and chemical properties. Banana peelsare chosen for the current experiment because of its easy availability and high cellulose content. The polymer produced by using the banana peel using glycerol could help in the formation of a biocomposite having paper-like characteristics with flexibility, pliability,etc. Various laboratoryanalyses like solubility, acid-base sensitivity, and biodegradabilityalong with fourier transform infrared (FTIR) and powder-x-ray diffraction (XRD) analysis would open up avenues for the prospective application of the polymer as a user-friendly biodegradable plastic. These bioplastics can play an important role in the market for sustainable use and can reduce the pollution caused by dumping of plastic and fruit wastes, thereby, providing aneco-friendly alternative.

Keywords: *Bioplastic, sustainable development, cellulose, polyhydroxyalkonoates, polyhydroxybutyrates, biodegradable, eco-friendly.*

AB:48

Karaya Gum and its Wide Applications

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Karaya gum, also known as Sterculia gum, is the dry exudate of *Sterculia urens* (Roxburgh), a large and bushy tree. The majority of commercial material is obtained from wild *S. urens* trees, indigenous to central and northern India and more than half of the gum is produced in the state of Andhra Pradesh. Other significant sources are from *S. setigera*, in Senegal and Mali, and minor supplies from *S. villosa* in Sudan, India, and Pakistan.

Karaya gum has been used commercially for approximately 100 years. Its use became widespread during the early 20th century, when it was used as an adulterant or as an alternative to 'Tragacanth gum'. However, Karaya gum possess physiochemical properties that are more beneficial than tragacanth. India is the largest producer and exporter of karaya gum.

Karaya gum is produced by charring or scarring the tree trunk and removing a piece of bark or by drilling holes into the trunk. The gum seeps from the scars and is collected, washed, dried, and then graded. A mature tree may yield 1 to 5 kg of gum per season. The gum karaya price fluctuates in the range US$ 2250–6000/ton according to grade. Fair average quality (FAQ) gum is about US $3000/ton.

Karaya gum is a complex, partially acetylated polysaccharide obtained as a calcium and magnesium salt. The polysaccharide component of karaya has a high molecular weight and is composed of galacturonic acid, beta-D-galactose, glucuronic acid, L-rhamnose, and other residues. It is used as a thickener and emulsifier in foods, as a laxative, as a denture adhesive and in seals. The gum has also been used in a variety of products, including cosmetics and lotions, and as a bulking agent. The gum has been used in ostomy care, as a base for transdermal delivery of medicines, and as a carrier for poorly soluble medicines. The gum has been tested as a biosorbent of toxic heavy metal ions.

Karaya gum has multiple application as food additive that can be used as a stabilizer, emulsifier and gelling agent. It has a great potency in pharmaceutical industry as adhesive, suspension, and tablet agent. It is economic, easily available and can be modified to obtain more accessible materials, presenting a wide advantage over synthetic materials.

AB:49

The Omnipresent, New-age Environmental Pollutants: Microplastics

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The study focuses on what microplastics are, how these substances entered the ecosystem and what its adverse effects are. Microplastics are the remnants of macroplastics and mesoplastics. These particles are let into the environment by disintegration of the synthetic polymeric compound plastic. Microplastics are wide-ranging; these are found not only on soil but, on water, in air, in the human placenta and in many marine animals. These particle enter the food web also, thus, have become a risk for food safety. According to studies, microplastic pollution is increasing day by day which is an alarming situation. Owing to its circumstances, it is of the essence to understand the impacts of microplastics not only in our surroundings but, in the trophic levels also. The study reports the harm caused by microplastics to the human body and how can we cope with this emerging pollutant.

Keywords: *Microplastics, Aquatic environment, Cadmium and Mercury uptake, Placenta, Extruded Polystyrene.*

AB:50

Plant based natural dyes from berries

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In life sciences, various staining techniquesare used to enhance contrast in samples at a microscopic level to identify various microbes, cells, organelles, membranes and chromosomes. Most of the stains used for this purpose include chemically synthesized dyes from cost effective petroleum sources, which shows rapid response and gives different variety of colors. But the main disadvantage is that, they cause skin allergies, and have toxic effects on exposure to human body. So it is very important to identify non-allergic, non-toxic and eco-friendly stains from natural sources. Generally stains are obtained from natural sources such as different parts of the plant like fruits, flowers, leaves and can be served as an alternative to synthetic stains.Recently, there have been a lot of reports on natural stains and dyes obtained frompigmented fruits like wild berries.Usually the juice extracted from the berries find use as dye for fabrics and cosmetics or as an ink. The natural dyes obtained from *Rivina humilis* (blood berry) and *Vaccinium myrtillus(*blue berry) have been reported to possess pigments which may be able to stain the microorganisms and plant tissues. The blood berries (*Rivina* sps) contain a red-pigment known as *rivianin* or *rivinianin* which gives color to the fruit, while blueberries (*Vaccinium myrtillus*) contains anthocyanin pigment which is a water soluble. This *rivianin* pigment has been found to be similar to *betanin* pigment found in beetroot (*Beta vulgaris*). In the present study, natural pigments from various berries have been extracted using organic solvents and tested for their efficiency in staining bacteria, fungi and plant cells.

Keywords: *Berries, Natural Dyes, Staining technique.*

AB:51

Photocatalytic Degradation of 4-Chlorophenol in Visible and Solar light over Ag doped and Bi doped TiO_2 nanoparticles

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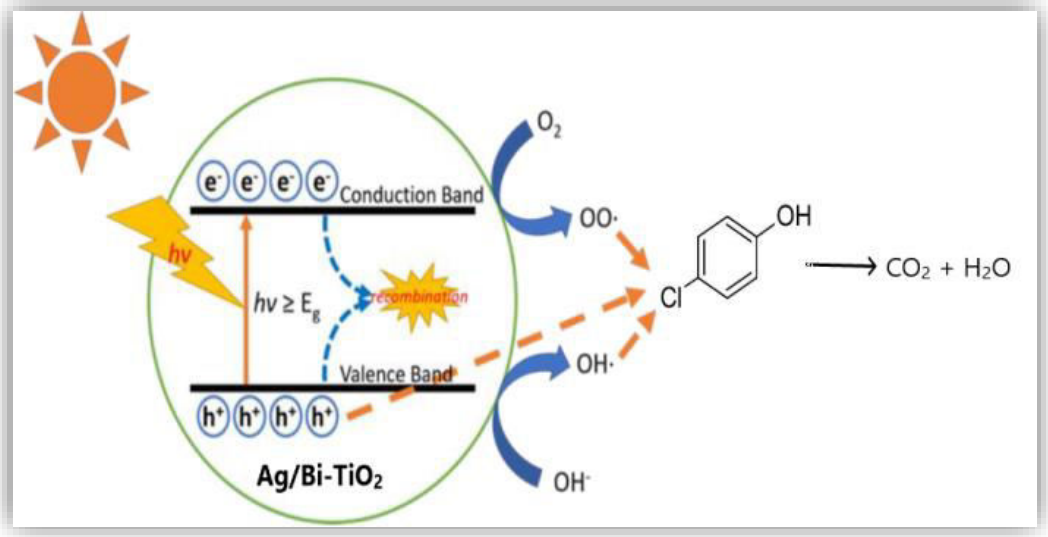
Chlorophenols are toxic, recalcitrant and hazardous compounds, normally present in soil, water and waste water as persistent pollutants because of its non-biodegradable nature.4-Chlorophenol is commonly found in the waste water of pulp, paper, pharmaceutical and dye stuff industries. The present study is focused on the doping of nano TiO_2 with Ag and Bi to widenthe visible light absorption window of TiO_2that can enhance its photocatalyticactivity. The Ag and Bi doped nano TiO_2 catalysts were synthesized by sol-gel method with 5wt% of the cation doping followed by calcination in air at 500ºC for 4 hours. These photocatalysts were then characterized by various adsorption and spectroscopic techniques viz., XRD, BET-SA, UV-Vis DRS, FT-IR, SEM-EDAX,TEM, XPS andPL techniques. The photocatalytic activity of the catalysts were studied in both visible and solar light clearly demonstrated a very high efficiency of the catalyst in degrading 4-Chlorophenol to an extent of more than 97% on Ag doped TiO_2 followed by Bi modified to an extent of 93% and bare TiO_2 up to68% with 50ppm of organic pollutant. The reusability test was conducted with most efficient catalyst (5wt%Ag doped TiO_2) for 4-chlorophenol degradation in order to check the stability of catalyst for practical application.



Photodegradation of 4-chloro phenol over Ag/Bi-nano TiO_2 Catalysts in visible and Sunlight

Keywords: *nano TiO_2, 4-chloro phenol, photocatalytic degradation, sunlight*

AB:52

Synthesis, biological evaluation of novel ternary metal complexes derived from dehydroacetic acid, bipyridyl and M (II) Cu, Co, Ni, and Zn as a prospective anti-microbial agent

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Nizam College Osmania University Hyderabad.

Ternary metal complexes of Schiff base derived from dehydroacetic acid, ethanolamine (DHEA), and bipyridyl with M(II)ions where M(II) = Cu, Co, Ni, Zn were prepared and characterized their molecular structures by elemental analysis, magnetic moment, UV, IR, Mass, TGA, and ESR. In the mononuclear molecule, the metal atom is bonded to ONO donor atoms from the Schiff base ligand and N, N donor atoms from the bipyridyl ligand. The geometry was found to be Octahedral. These complexes were evaluated against bacterial and fungal strains. Considerable activity is observed.MIC values of the complexes have been comparable with regular drugs as Tetracycline and Amphotericin B.

Keywords: *Dehydro acetic acid, bipyridyl, mixed ligand complexes.*

AB:53

Synthesis of Mesoporous Alumina with High Surface Area as an adsorbent for CO_2 gas

V. Shashikala*, A. Ramesh

Mesoporous Alumina (aluminium oxide – Al_2O_3) materials with high surface area and a narrow pore size distribution were synthesized using a simple co-precipitation method. In this method alcohols (ethanol and butanol) and water were have been used as solvents and di ethanol amine (DEOA) using as precipitating agent. The precipitated cake was washes with ethanol to neutral pH followed by drying and calcinations at different temperatures from 200ºC to 600ºC. After calcination physical properties of such as powder X ray analysis, nitrogen adsorption to get BET surface of all the samples were analysed. XRD analysis conforms the gamma alumina phase (JCPDFS number 895898). A very high surface area around 400 m^2/g was obtained for the sample calcined at 300 ºC. Pore size distribution and pore volume are increasing with increase in the calcinations temperature.

Key words: Synthesis, Alkanolamine, gamma – Alumina, High surface area (~ 400 m^2/g), Mesoporosity

AB:54

Bismuth (III)-Catalyzed synthesis of 2-substituted Benzothizoles

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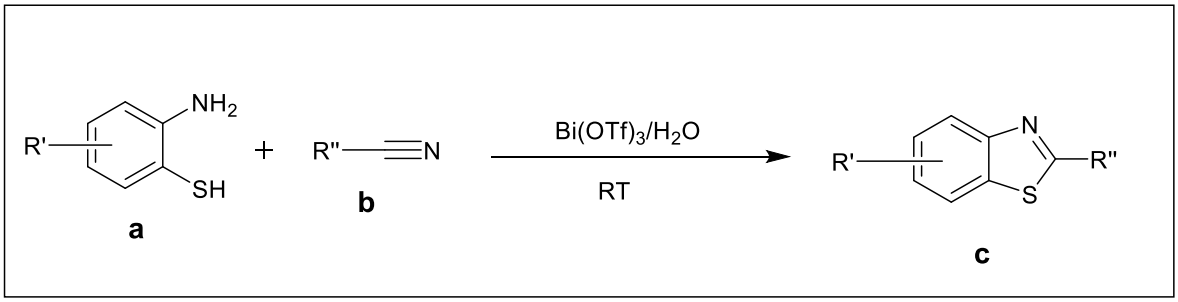
Osmania University, Hyderabad-500095, India

Abstract: A simple and efficient protocol has been developed for the synthesis of 2-substituted benzothiazoles from simple and readily available 2-amino thiophenols and nitriles using $Bi(OTf)_3$ as catalyst. With this method 2-substituted benzothiazoles were produced in excellent yields in short reaction times under mild and green conditions. Owing to its unique catalytic properties, bismuth (III) triflate has been extensively used for a plethora of organic transformations and water as a green solvent, for economical and safety reasons has become a substitute and an alternative environmentally benign solvent in organic synthesis. We found that $Bi(OTf)_3/H_2O$ as a simple and efficient catalyst for the synthesis of Benzothiazoles. The reaction is clean and high yielding.

Key words: Benzothiazoles, 2-aminothiophenols, nitriles, green solvent



ABSTRACTS OF ORAL PRESENTATIONS

UNIVERSITY COLLEGE FOR WOMEN

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A Constituent and Autonomous College of Osmania University, NAAC accredited with 'A' Grade

TWO DAYS VIRTUAL INTERNATIONAL CONFERENCE on CHEMICAL ADVANCES FOR SUSTAINABLE DEVELOPMENT

Dates: 12th and 13th April 2022, Time: 10.00 AM to 5.00 PM

EVALUATORS FOR THE TECHNICAL SESSIONS

Dr. M. Kavitha
Assistant Professor
Dept. of Chemistry
UCS, OU

Dr. A. Hari Padmasri
Associate Professor
Dept. of Chemistry
UCS, OU

Prof. G. Vijaya Charan
Professor
Dept. of Chemistry
UCS, OU

Prof. K. Girija Mangathayaru
Professor
Dept. of Chemistry
Palamuru University, Telangana

Date: 12th April 2022, Tuesday	**2.15 PM – 4.30 PM**	**Technical Session– I**
Date: 13th April 2022, Wednesday	**12.10 PM – 1.40 PM**	**Technical Session– II**
	2.40 PM – 3.40 PM	**Technical Session– III**

Organised by: Department of Chemistry, UCW

OP:01

Mxenes/WO_3 composites for gas sensing applications

Pooja Bajaj and Manorama V Sunkara *

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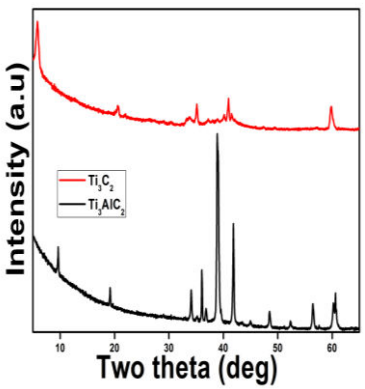
Mxenes with general formula $M_{n+1}X_nT_x$ where M represents transition metals (like Sc, Ti, V, Cr, Zr, Nb, Mo and Ta), X is C or N, T the surface terminal groups (like O, F, and OH), and n=1,2,3 are a new family of 2D materials that have attracted a great deal of attention in different areas of Materials Science. The excellent properties of these materials like high specific surface area, conductivity, flexible components, and variable layer thickness make them good candidate materials for applications in sustainable energy devices like in sensors, energy storage, hydrogen generation, water purification devices etc.

Despite the excellent properties that Mxenes exhibit, the major drawbacks these materials possess is they are not stable in ambient conditions. This instability is because of the oxidation that leads to disruption of material properties, which limits its application potential.

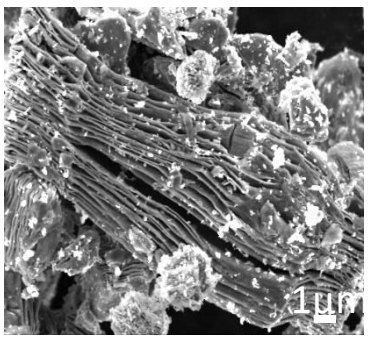
Miniaturized flexible gas sensors are getting popular over rigid ceramic sensors because of their low cost, biocompatibility, and their ability to be integrated into smart wearable and portable electronic devices.

The present study is an attempt to overcome the above challenges by making composites with semiconducting oxides which is anticipated to impart stability to Mxenes and make these materials amenable for applications in gas sensing.

A synthesis protocol has been established to obtain composites of Mxenes with WO_3, the study presents the material properties evaluation by PXRD, FESEM and TGA that have been improved by making the composites and demonstrated their performance when used as a gas sensing material.



PXRD of Ti_3AlC_2 & Ti_3C_2



FESEM image of Ti_3C_2

OP:02

TiO_2 Nanocomposites: A Comparative Study with TiO_2 Nanoparticles using various Characterization Techniques

M. Vijayatha, B.Vijayalaxmi,Md.Sajeeda and A. HariPadmasri*

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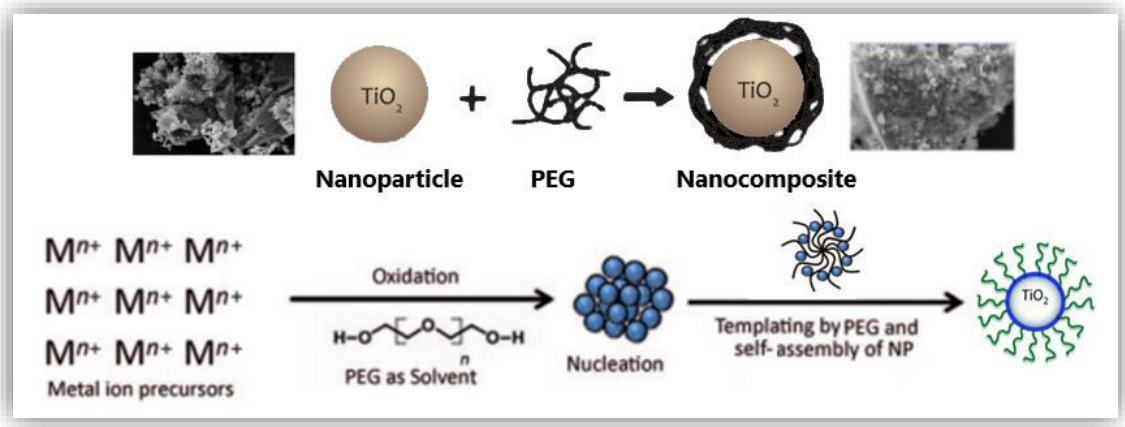
Nanomaterials are sought to be very interdisciplinary in nature that overlaps the field of Nanotechnology and Nanoscience.Our study is on the surface modification of TiO_2 Nanoparticle (NP)using Polyethylene Glycol (PEG) which is the widely used polymer due to its non- toxic,hydrophylic, biodegradable and biocompatiblenature.Titaniais considered to be one of the most versatile materials in its nanoformwhich has led us to study its synthesis as pure TiO_2 nanoparticles and modification of thus formed TitaniaNPsby dispersing it in polymer matrix forming Polymer Nanocomposite.Sol-Gel procedure was used as experimental methodfor synthesizing TiO_2NPscarried by PEGylationusing PEG 4000.On the basis of modification process,the effect of PEGon the size and morphology of prepared NPswasthen evaluated and compared using characterization techniques like UV-Vis DRS, XRD, FT-IR & Raman spectroscopy, SEM-EDX and BET Surface area analysis.In the future,titania – based nanomaterials are expected to open new approaches for demonstrating their outstanding applications in diverse field.



KEYWORDS: *Nanocomposite, PEGylation, biocompatible,Scanning Electron Microscope, X-RayDiffraction.*

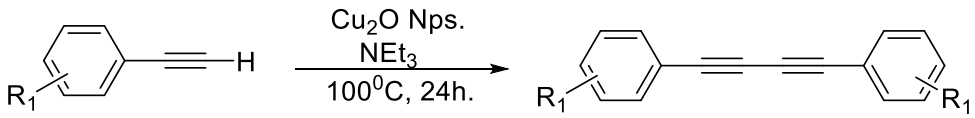
OP:03

Template free synthesis of stable Cu_2O nanoparticlesand its application in Glaser – Hay coupling

A. Ramesh, V. Shashikala*

Template free synthesis of Cu_2O nanoparticles wereprepared in propanol and water using as a solvent at room temperature under ambient air conditions. Redox method was used, in this process alkanolamines are used as stabilizing agents.It was proposed that metallacyclic co-ordination stability of ring type between the ionic Cu and alkanolamine on to the surface of Cu, resulting in the superior stability of Alkanolamine-Cu_2O Nps. Synthesized Cu_2O Nps were characterized by using various analytical studies like XRD, XPS, SEM, EDS. Thussynthesized Cu_2O acts as a robust and an efficient catalyst for construction of 1,2,3-triazole ring compounds and C-C bond formation in Glaser-Hay coupling reactions.

Keywords: Template free, Alkanolamines, stable Cu_2Onanoparticles, Glaser – Hay coupling.



Phenylacetylene 1,4-diphenylbuta-1,3-diyne

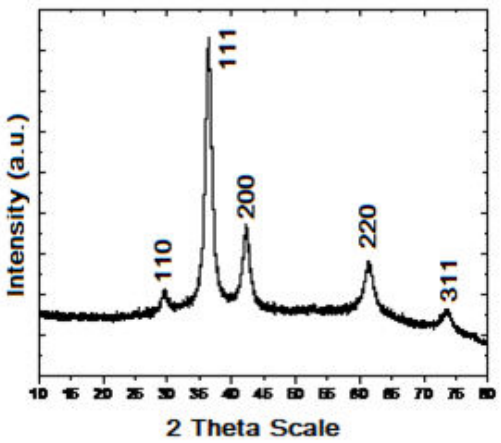


Figure 1: X Ray diffraction patterns of Cu2O

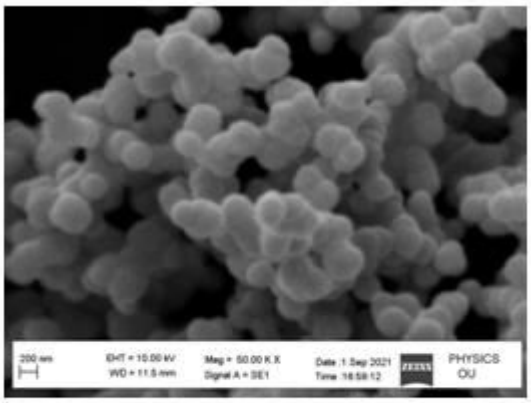


Figure 2: SEM images of Cu2O

OP:04

Synthesis and Characterization of Nanoparticles Heterocyclic Compounds

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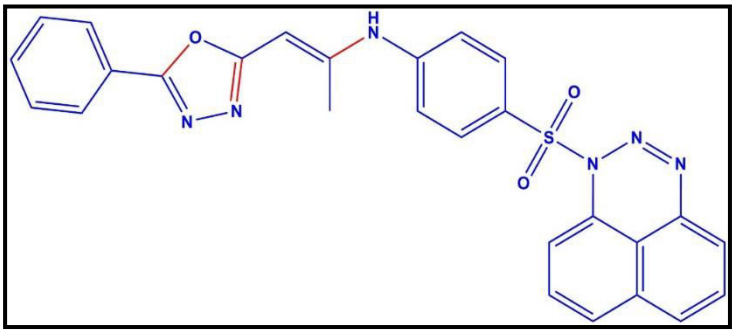
Abstract:
The reaction between 4-((1H-naphtho[1,8-de][1,2,3]triazin-1-yl)sulfonyl)-N-(4(hydrazinyloxy)-4-oxobut-2-en-2-yl)aniline and benzaldehyde in the presence of iodine yielded novel heterocyclic compound,4-((1H-naphtho[1,8-de][1,2,3]triazin-1-yl)sulfonyl)-N(1-(5-phenyl-1,3,4-oxadiazol-2-yl)prop-1-en-2-yl)aniline (NTOD). The novel synthesized compound was characterized by spectroscopic method. In aqueous media novel synthesized heterocyclic compound NTOD's nanoparticles prepared by re-precipitation method. These nanoparticles characterized by using UV-Vis spectrophotometer and scanning electron microscope (SEM). SEM shows the size of the nanoparticles were around 70-100 nm. There is head to head alignment (J aggregate) of the molecules of NTOD during the aggregation which was confirmed by the maximum of absorption spectrum of the dispersed nanoparticles is red shifted by 5 nm from the molecular absorption spectra of the NTOD in the solution.



Keywords: *Heterocyclic compound, Nanoparticles, Oxadiazoles, Prparation, spectroscopic data analysis.*

OP:05

Ascaridia galli (chicken nematode) as a source for Nanoparticle and Nanofiber

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Green synthesis of nano particles and nanofiber gained relevance in recent times. Ideally nanoparticles and nanofiber are made from metallic sources. However, in recent times, there are reports of drastic side effects about the use of metallic nanoparticles in biology and medicine. In this context, it has become more relevant to explore and identify, more natural and biofriendly and effective alternative to metallic ones. There are instances, where, nano particles and nanofibers, and many other nano components, have been synthesized from more natural sources, such as bacteria, different species of algae and also from fungi. However, not many have attempted to synthesize nanoparticles, from unusual sources such as nematodes, the intestinal parasites of animals and humans. For the first time, in the present study it was attempted to synthesize nanoparticles and nanofiber from the intestinal nematode of chicken, *Ascaridia galli*. The parasites, were extracted and isolated from the chicken intestines, they were later processed for the synthesis of nanoparticle and nanofiber. It is quite evident that nanoparticles, synthesized from a natural source are more appealing as they are both eco friendly and inexpensive. Parasite, measuring approximately 30-80mm in length were carefully removed from chicken intestines and later processed for the synthesis of nano particle and nano fiber. Nanoparticles were synthesized using the method of acid hydrolysis and nanofiber was prepared using electro spinning technique. The nanofibre which was synthesized, was hydrophilic in nature, and measured about 6cm x 3cm in size. Scanning electron microscope (SEM)images of nanoparticle revealed a diameter of 48.46nm-20µm and the nanofiber diameter was found to be between 88nm-2 µm, thus matching to the average standard size of nano particle and nanofiber. As the intestinal parasites, are capable of evading host immunity and can easily amalgamate with the host tissues, without triggering any antagonism, therefore can be used frequently in biology and medicine. As these nanoparticles and nanofiber, are synthesized using a parasite,(a living source) it can easily be degraded after the use, and may be considered as a suitable alternative to metallic nanomaterials.

Key words: *Nanoparticle , nanofiber, Ascaridia galli. electro spinning, SEM, chicken nematode*

OP:06

Plant mediated synthesis of SnO_2 nanostructuresfor methyl orange degradation

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We report herewith additive-free, environmentally sustainable, rapid and phytosynthetic way for the fabrication of nanostructures (NSs) of UV active SnO_2 photocatalyst (E_g= 3.59 eV) employing *Syzygium cumini*(SC) leaf extractwhich acts as a reducing and stabilizingagent. The preparedSnO_2nanostructures were characterizedby host of different techniques such as Xraydiffraction (XRD), diffuse reflectance spectroscopy (DRS),fourier transform infrared spectroscopy (FT-IR) and Brunauer-Emette-Teller (BET) surface area analyzer. The XRD patternconfesses that the diffraction peaks are in good agreement with tetragonal rutile $SnO_2$and the average crystallite size was found to be 3.2nm which is calculated from the X-ray line broadening of peaks by using Scherrer's formula. The DRS absorption spectrum was used to calculate band gap of material and it isfound to be 3.59 eV.Sn-O-Sn bond confirms at 560645 cm^{-1} in FTIR suggests the formation of SnO_2. The surface area of material was determined using BET surface area analyzer and it was found to be 58 m^2-g^{-1}. SnO_2nanostructures were subjected to photocatalytic degradation of methyl orange (MO) under UV light. Thephotodegradation efficiency of MO was found to be 88%within 180 min under UV light radiation.

Keywords: *Plant mediated, SnO_2nanostructures, photodegradation*.

OP:07

Synthesis And Characterisation Of Nanoparticles Using Green Extracts- A Review

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In materials science, "green" synthesis has gained extensive attention as a reliable, sustainable and eco-friendly protocol for synthesizing a wide range of materials/nanomaterials including metal/metal oxides nanomaterials, hybrid and bio inspired materials.Biomolecules present in plant extracts can be used to reduce metal ions to nanoparticles in a single-step green synthesis process.Nanoparticles have been developed with progress in nanotechnology and applied to wide range of fields such as drug/gene deliveryand playa key role as a catalyst in synthesis of organic compounds.Synthesis of nanoparticles by biological methods using microorganisms, plant extracts and enzymes have attracted great attention recently.This biogenic reduction of metal ion to base metal is quite rapid and can be readily conducted at various temperatures, pH and concentrations. Synthesis mediated by plant extracts is environmentally benign and have been successfully used in making nanoparticles.. The reducing agents involved include the various water soluble plant metabolites such as alkaloids, phenolic compounds, terpenoids and co-enzymes.

In this review, we summarized the fundamental processes and mechanisms of green synthesis approaches, especially for metal and metal oxide of gold (Au), silver (Ag), copper oxide (CuO), and zinc oxide (ZnO)] nanoparticles using natural extracts. Importantly, we explored the role of biological components, essential phytochemicals such as flavonoids, alkaloids, terpenoids, amides, and aldehydes as reducing and capping agents. The spectroanalytical techniques such as UV-Visible spectrophotometer, FT-IR, XRD, TEM,SEM,Particle size analyzer and Zeta potential are employed for the characterization of synthesized nanoparticles. The article also reflects the applications of nano particles in terms of antimicrobial activity, catalytic activityand environmental remediationsuch as removal of pollutants, dyes and heavy metal ion sensing.

Keywords: *Green extract, Nanomaterials,Zeta potential, SEM and TEM*

OP:08

Application of Magnetic Nano - Fe_3O_4 in Environmental Forensic and Food Sciences

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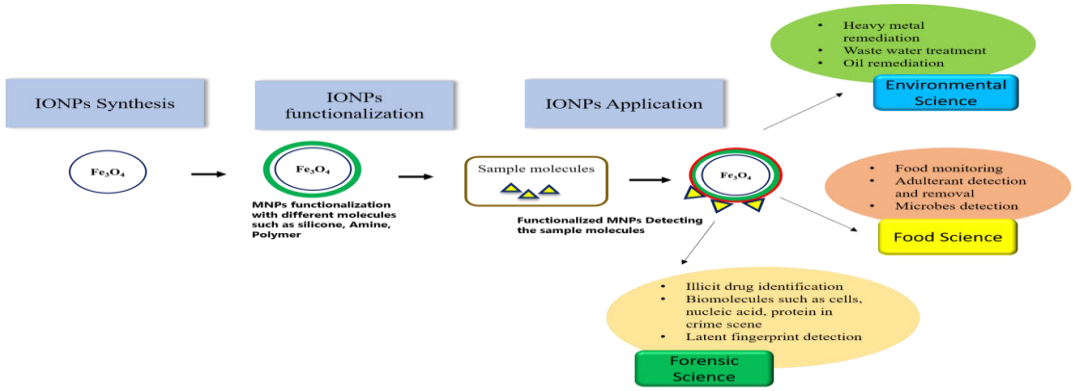
The diversity in the application of iron nanoparticles (IONPs) is quite remarkable that draws attention among researchers. The basis for their diversity lies in their exceptional properties apart from the typical nano properties, that eventually creates space for upcoming and most required fields. Therefore, the present paper discusses about the significant role of IONPs in disciplines like forensic, food and environmental. IONPs aids in detecting the presence of the toxic compounds during food manufacturing, identifying the harmful adulterants in food items and deleterious pathogens. IONPs can also assist in solving crimes by identifying the sample types accurately such as n detection of illegal drugs and cells (sperm and epithelial cells) that are difficult to differentiate, also aid in making latent fingerprints visible. Among the new technologies IONPs also have great part in reviving the polluted environment by remediating heavy metals from soil, water, treating waste water, removing oils from sea waters and so on. Hence, in upcoming days it could be anticipated that IONPs can contribute to real-time applications in various disciplines. The special properties of Nano Fe_3O_4 among the nanoparticles has created special attention in researchers of different fields. Considering their typical property of super magnetism, it creates spaces for some special fields like environmental, forensic and food sciences that have been taken for discussion in the present paper. Nano Fe_3O_4 helps in detecting the presence of the toxic compounds during food manufacturing, identifying the harmful adulterants in food items and deleterious pathogens. Nano Fe_3O_4 can also assist in solving crimes by identifying the sample types accurately such as n detection of illegal drugs and cells (sperm and epithelial cells) that are difficult to differentiate otherwise, also aid in making latent fingerprints visible and aid in explosive powder detection that are usually difficult. Among the new technologies Nano Fe_3O_4 also have great part in reviving the polluted environment by remediating heavy metals from soil, water, treating waste water, removing oils and microplastics from sea waters and others that otherwise can cause havoc to living organisms. Hence, in upcoming days it could be anticipated that Nano Fe_3O_4 can contribute to real-time applications in various disciplines.



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

References

- Farouk, F. et al. "Detection of Acinetobacter Baumannii in Fresh Produce Using Modified Magnetic Nanoparticles and Pcr." *Anal Biochem*, vol. 609, 2020, p. 113890, doi:10.1016/j.ab.2020.113890.
- Huang, Rui and Yuting Zhang. "Synthesis of Fe3o4@Gsh-Pt Ncs Core-Shell Microspheres for Latent Fingerprint Detection." vol. 91, no. 12, 2018, pp. 1697-1703, doi:10.1246/bcsj.20180168.
- Lee, Seon-Yeong et al. "Tryptamine-Functionalized Magnetic Nanoparticles for Highly Sensitive Detection of Salmonella Typhimurium." *Analyst*, vol. 146, no. 8, 2021, pp. 25592566, doi:10.1039/D0AN02458A.
- Madhusudhana Reddy, P. et al. "Robust Polymer Grafted Fe3o4 Nanospheres for Benign Removal of Oil from Water." *Applied Surface Science*, vol. 368, 2016, pp. 27-35, doi:https://doi.org/10.1016/j.apsusc.2016.01.250.
- Seddaoui, Narjiss and Aziz Amine. "A Sensitive Colorimetric Immunoassay Based on Poly(Dopamine) Modified Magnetic Nanoparticles for Meat Authentication." *LWT*, vol. 122, 2020, p. 109045, doi:https://doi.org/10.1016/j.lwt.2020.109045.

OP:09

Antioxidant and catalytic activity of *Biogenic* NiO nanoparticles from, *Terminalia Chebula* Aqueous Extract

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Nowadays, the biological synthesis of nanoparticles attains researchers' interest in removing hazardous pollutants from water. Due to eco-friendliness, coast effective, non-hazardous, and avoids the usage of catalyst and stabilizing agents. Herein, the *Terminalia Chebula*-NiO NP nanoparticleswas prepared at ambient conditions by using aqueous *Terminalia Chebula* fruit extract. *Terminalia Chebula*fruit extract contains polyphenolic compounds, terpenoids, carbohydrates, and flavonoids, which can be responsible for the nucleation of NM in biological synthesis. The resulted *Terminalia Chebula*-NiO NP was characterized via UV, FTIR, zeta potential, XRD, EDX, SEM, and TEM. The UV and XRD analysis confirmed the formation and cubic crystalline nature of *Terminalia Chebula*-NiO NP, receptively. FTIR, EDX, and Zeta potential confirmed the functional groups, elemental composition, and surface charge. Additionally, they explain that phytochemicals were responsible for the reduction and stabilization of *Terminalia Chebula*-NiO NP. The average size of the *Terminalia Chebula*-NiO was identified to be 14.08 nm and spherical in shape with TEM.In addition, antioxidant and catalytic activities performance of the NiO NPs were investigated. The Terminalia Chebula-NiO NPs showed highest antioxidant activity at 100µg/ml as 63.46, EC 50% as 41.73µg/ml against DPPH and completely degraded Congo red dye within 20 mins, overall, the experimental results suggested that the nanoparticle developed could be helpful for Industrial applications.

Keywords: *Antioxidant; Biosynthesized; Catalytic; Eco-friendly, Photochemical.*

OP:10

Impact of beehiving practices and processing on the chemical composition of honey:-Comparative study

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Honey is a sweet liquid obtained from nectar collected by beehives from flowers. The aroma of honey will vary depending on the types of flower sources used to harvest nectar. Honey contains a complex chemical composition that differs from the botanical source. Sugar, organic acids, mineral salts, vitamins and enzymes are the main components of honey. Honey is better known for its cough-relieving qualities, but it also promotes blood circulation and the assimilation of calcium and magnesium into the bone structure. It has antioxidant and antibacterial properties that keep the wound moist and its high viscosity aids in the appliance of a protective barrier to prevent contagion. The purpose of this study was to study the effect of floral origin on the physicochemical characteristics and chemical composition such as calcium, iron, glucose and vitamin C . Three different commercial brands were taken and analyzed honey and compared to that of organic honey. Physicochemical constituents were identified using AQAC methods. The physicochemical parameters are -viscosity, moisture content, free acidity, Total ashsoluble ash, insoluble ash and sulfated ash were determined. The minerals were determined using different titrimetric analyses. Back titration method for estimation of calcium, permanganometry for estimation of ferrous and colorimetric analysis for estimation of vitamin C. Direct titration method for estimation of reducing sugar- glucose. According to the analyses, organic honey had higher viscosity and moisture content than brand honey. Total ash, ferrous, and calcium content appear to be higher in branded honey. On the other hand, organic honey appears to be high in reducing sugar and vitamin C. Organic honey has a high level of free acidity, which may cause storage and stability issues over time

Key words: *Honey, Physiochemical properties, minerals, reducing sugar*

OP:11

Analysis of Physico- Chemical properties of multi ingredient multipurpose flour with an extended shelf life for pre diabetic and diabetic population

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Background and objectives: Carbohydrates play a vital role in addressing human requirement for energy from food along with shelter and clothing to modern world. Changed life style has led to many disabilities and diseases, most commonly obesity and diabetes. Carbohydrate based nutraceuticals have been claimed to have effective disease preventing, curative and health promotive virtues. The raising importance of dietary fibres has led to the concept of multi grain Atta. After an insight into the concept a need for multipurpose multi grain Atta with functional foods and nutraceuticals is developed. The use of functional foods and their bioactive components have been considered as a new approach in the prevention and management of diabetes and its complications. The significance of carbohydrates and their correlation with diabetes prompted us to develop and promote flour with low glycaemic index foods and spices with potential to bring hypoglycaemic effect and extended shelf life.

Materials and Methods: Three cereals, three millets, two oil seeds, three legumes and five spices were used in a specific proportion to develop the flour. Different processing techniques were adopted such as soaking, sprouting, roasting and grinding. The physico chemical characterisation was carried out in which the Moisture content, total ash value, Sulphated ash, Acid insoluble ash were carried out the acid values which indicate the stability of the sample were also carried out adaptability of flour was tested by developing different foods using different methods of cooking such as steaming, shallow frying and deep fat frying, and baking. This is assessed for the degree of acceptance of the product through sensory evaluation.

Results: The flour showed good functional properties such as water absorption, plasticity, gelatinization with acceptable palatability. Chemical analyses were carried out for proteins and fat where in protein content was observed to be 16% and above. Fat content though high is mostly from plant steroids. Shelf life of the flour without any preservative is beyond two years

Conclusion: The technology for development of flour is consumer friendly with minimum understanding. There is increasing demand by patients to use the natural products. The multi-purpose nature of the flour opens way for food innovations for target population with flexibility to be used in modern processing techniques such as extrusion. However the biochemical mechanism and physiological action of some substances involved needs further studies.

Key words: *Multi grain, multi-purpose, Diabetes and innovation*

OP:12

Green synthesis, DNA Interaction, molecular dynamics simulation, molecular docking,*in vivo* anti-inflammatory,biological and thermal studies of Fe(III), Co(II), Ni(II) and Cu(II)complexes of (E)-2-(1-((2-fluorophenyl) imino)ethyl) phenol Schiff base.

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Microwave assisted reactions, as current approach of synthesizing Schiff base and metal complexes have given a new direction in the field of green chemistry.Series of transition metal complexes, $[Fe(HL)_2Cl(H_2O)]$**(1)**, $[Co(HL)_2]$**(2)**, $[Ni(HL)_2]$**(3)** and $[Cu(HL)_2]$**(4)** with a Schiff base ligand **(HL)**derived from o-Hydroxyacetophenone and 2-Fluoroanilinehave been synthesized and characterized by analytical and spectral studies. Structural and bonding parameters have been deduced, which revealed octahedral geometry for complex **1** and square planar geometry for complexes (**2**), **(3)** and **(4)**. Coats-Redfern calculations for deriving thermodynamic properties, suggest that all the complexes are non-spontaneous and thermally stable. DNA binding studies revealed intercalation binding mode,while intrinsic binding constant(K_b), S*tern-Volmer* quenching constant(K_{sq}) support high binding abilities. The nuclease activity of the metal complexes was carried out by gel electrophoresis using CT-DNA. Docking studies were done using Accelry's Discovery Studio 2.1 program to understand binding affinities. MD simulation, carried in order to analyze the stability of ligand and human Topoisomerase I (PDB ID: 1T8I) complex for 100 ns using the Desmond 2020.1 from Schrödinger, LLC revealed stable conformation of theligand.*In vivo* carrageenan induced inflammation studies in paw volume were carried out in rats and results show a higher rate of edema inhibition for complex **4**. *In vitro* cytotoxicity and antimicrobial assay revealed higher cytotoxic and microbial activity for complex **4**over other complexes and the ligand.

Key words: *DNA binding, invivocarrageenan, in vitro cytotoxicity, MD simulation,docking.*

OP:13

Microwave synthesis, characterization, Antioxidant activity studies, DNA , Protein binding& antimicrobial investigations of novel cobalt complex of 2-(1H-Tetrazol-5-yl) Acetohydrazide.

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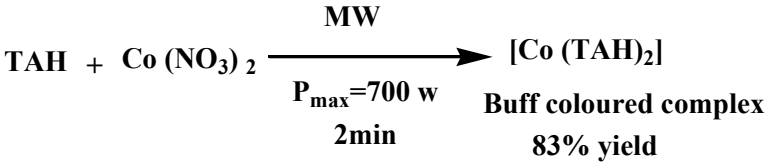
Novel Co (II) complex of 2 –(1H-Tetrazol-5-yl) Acetohydrazide (TAH) was synthesized by eco-friendly micro-wave assisted synthesis. Its spectral characterization was done using IR, UV and LCMS techniques. Based on spectral information, the geometry of the complex was predicted as octahedral. This complex was investigated for its radical scavenging ability, DNA, protein binding& antimicrobial propensities. This complex displayed mild antioxidant activity, and appreciable binding towards CT-DNA & Bovine albumin. Antimicrobial investigations revealed potent bactericidal activity against staphylococcus aureus, compared to control streptomycin. All the activities were compared with that of nascent ligand. It was observed that coordination with Cobalt has led to enhancement of all the activities , including antimicrobial activity.



OP:14

Green Synthesis of 3,5-disubstituted 1,2,4-oxadiazoles from Amidoximes and N-Hydroxyl Phthalimide Esters using spinach juice

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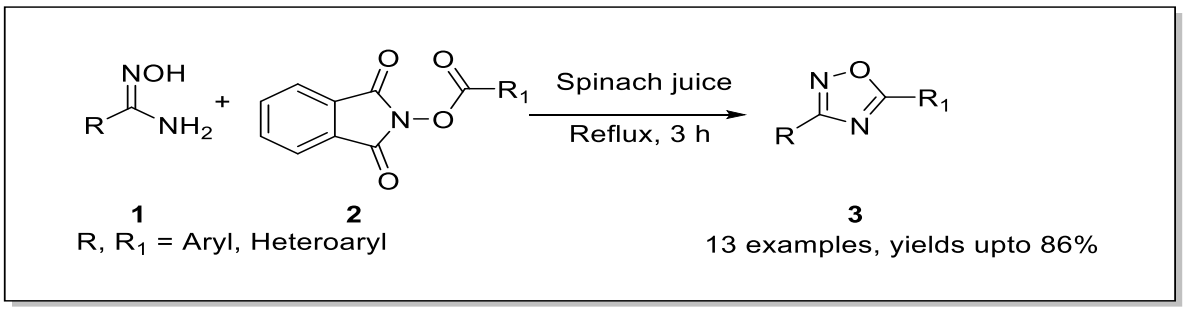
Oxadiazoles are one of the privileged heterocyclic moieties which are present in several natural products, pharmaceuticals. In particular,1,2,4-oxadiazoles exhibit various biological activities like, anti-fungal, anti-tubercular, anti-bacterial, anticancer and pharmacological applications like sphingosine-1-phosphate-1 (S1P1) receptor agonist, muscarinic agonist, serotoninergic antagonists, monoamine oxidase inhibitor anti-inflammatory, Anaesthetic, Vasodilator, anthelmintic, anti-allergic, antiplatelet activities etc. Due to their wide range of applications several methods have been reported for the synthesis of 1,2,4-oxadiazoles, but these methods are limited by the use of transition metal catalysts, additives and solvents which are environmentally unfriendly. So there is a need for the development of a green protocol for the synthesis of 1,2,4-oxadiazoles. In this context we report a green protocol for the synthesis of 3,5-disubstituted 1,2,4-oxadiazoles from easy accessiblestarting materials like amidoximes and N-hydroxypthalimide esters using spinach juice as green solvent under reflux for 3 h without any catalyst. In this reaction spinach juice is not only used as a green solvent but also used for the acceleration of the reaction. By green protocol we restrict the formation of byproducts. All the functional groups tolerated well and about 13 derivatives were synthesised in good to excellent yields.



Scheme: Synthesis of 3,5-disubstituted 1,2,4-oxadiazoles

Keywords: *1,2,4-oxadiazoles, spinach juice, amidoxime, N-Hydroxyl phthalimide ester, green synthesis.*

OP:15

Diels Alderase – A thriller story of nature

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Diels-Alder reaction is a [4+2] cycloaddition reaction between a conjugated diene and dienophile molecules. Stereo selective Diels-Alderreactions have been of interestto organic chemists for several decades because of application in drug manufacturing. Typically, DielsAlder reactions by chemical methods result in multiple stereoisomers which further needs to be separated. Due to the complicated processes in the purification and loss of precious material in the form of unwanted isomers, alternate stereo specific methods have been sort. In addition to chemical catalysts, biological catalysts also have been explored.

Some proteins have been shown to carry out intra-molecular Diels-Alder reactions in the biosynthetic process of macrolides. However, there have been limited efforts in exploring the proteins that carry out inter molecular Diels-Alder reactions. Given their importance, we have explored several microbial genomes and selected four proteins that are predicted to have a b-barrel structure and right cavity size to carry out inter molecular Diels-Alder reaction on synthetic substrates.

Initial data suggests that of the possible four isomers, recombinant DielsAlderases synthesize a single isomer. We have carried out detailed biochemical, X-ray crystallographic, mass-spectrometric and chromatographic studies to understand the molecular basis of the reaction. Details of the current understanding will be discussed during the presentation.

Keywords: *Biocatalysis, Diels Alderases, b-barrel protein, Diels-Alder reaction*

OP:16

Pd/SBA-COOH is a green catalytic boat for the production of H_2 at Room Temperature in aqueous media

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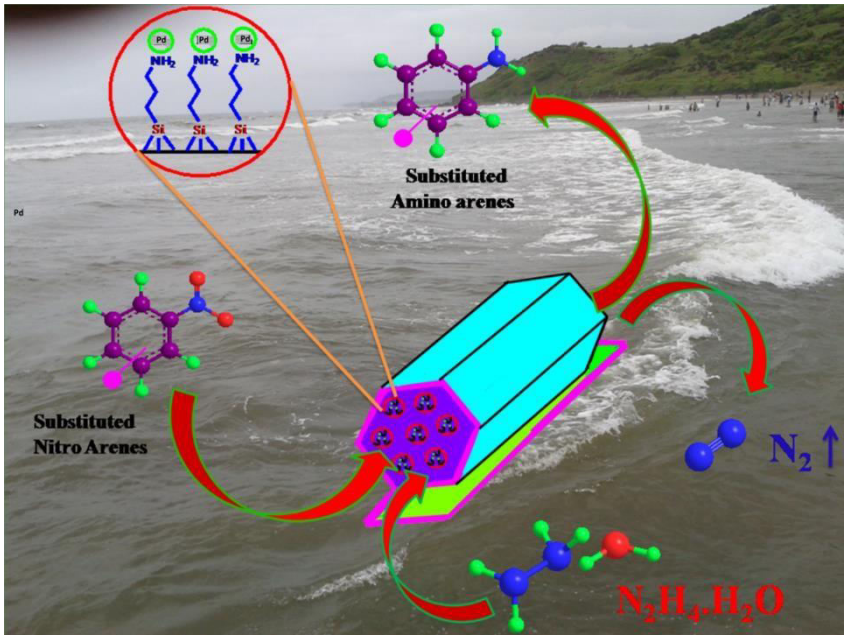
A room temperature aqueous medium Hydrogen production from hydrous hydrazine and its *insitu* utilization for the reduction of aromatic nitro compounds to its corresponding amines has been delineated over PdNPs/SBA-15catalytic system for the first time. The catalyst have been synthesized using functionalized SBA-15 (SBA-COOH) as support, palladiumacetate as a Pd precursor and characterized by XRD, N_2-adsorption-desorption isotherms, Transmission Electron Microscopyand FT-IRtechniques.



OP:17

Chances and Confronts in utilization of CO_2

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Focusing on converting the output generated from fossil fuels to economies gives a buoyant picture of achieving carbon neutrality. By integrating the energy and materials,a framework for carbon neutrality can be achieved. Balancing the CO_2 emission could be the leading global environmental goal of the 21st century.The assessment on carbon dioxide sequestering highlights the challenges for capture and storage of carbon to reduce CO_2 emissions from major sources. The most advanced and emerging concepts for CO_2 separations include adsorption and absorption. Reducing CO_2 emissions have been reported in literature by methods like low carbon economy, carbon transition, decarbonization, low carbon development, carbon neutrality, zero net carbon emissions and carbon footprint. The best practice for organizations and individuals seeking carbon neutral status entails reducing carbon emissions first so that only unavoidable emissions are offset. Carbon neutral status can be achieved in two ways 1)by balancing carbon dioxide released into the atmosphere from burning fossil fuels, with renewable energy and 2)by carbon offsetting by paying others to remove or sequester 100% of the carbon dioxide emitted by buying carbon credits to remove them through carbon trading. The central idea of this paper is to seek to treat CO_2 as a commodity rather than accountability.

OP:18

Green synthesis of copper nanoparticles using aqueous alternantera sessilis (linn.) Leaf extract and the study of antioxidant, photo catalytic and antibacterial study.

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In the present study, phyto-fabricated Copper nanoparticles (CuNPs) were prepared from aqueous leaf extract of *Alternanthera sessilis* by a facile, economic, and eco-friendly approach. The facile phytofabrication of CuNPs was confirmed by UV-visible spectroscopy with characteristic peak around λmax of **560-570nm**, FTIR spectroscopic analysis and Zetapotential analysis confirmed that *TC*-Cu NPs were synthesized by phytoconstituents of *Alternanthera sessilis*aqueous leaf extract, negative charge (-29.1 mV) reveled the formation stable Alternanthera sessilis-Cu NPs. The XRD pattern showed that synthesized *Alternanthera sessilis*-Cu NPs were crystalline in nature with FCC structure. The SEM images depicted that *Alternanthera sessilis*-Cu NPs were irregular in shape. The spherical shape and size of about 3-12 nm were revealed by TEM analysis. The biogenic Cu NPs demonstrated fascinating dose dependent antioxidant activity with EC50% as 68.73g/ml, and highest activity as 58.36 at 100 g/ml, as well as significant Photo catalytic activity against Congo red dye, which was completely degraded after 20 minutes. Furthermore, the studies revealed that Cu NPs displayed greater antibacterial efficacy against Gram negative bacteria than Gram positive bacteria.

Key Words: *Alternanthera sessilis, Metabolites, Biosynthesis, Copper Nanoparticls , Antioxidant.*

OP:19

Synthesis of Sulfur Doped Graphene and its Electrocatalytic Application for Hydrazine Determination

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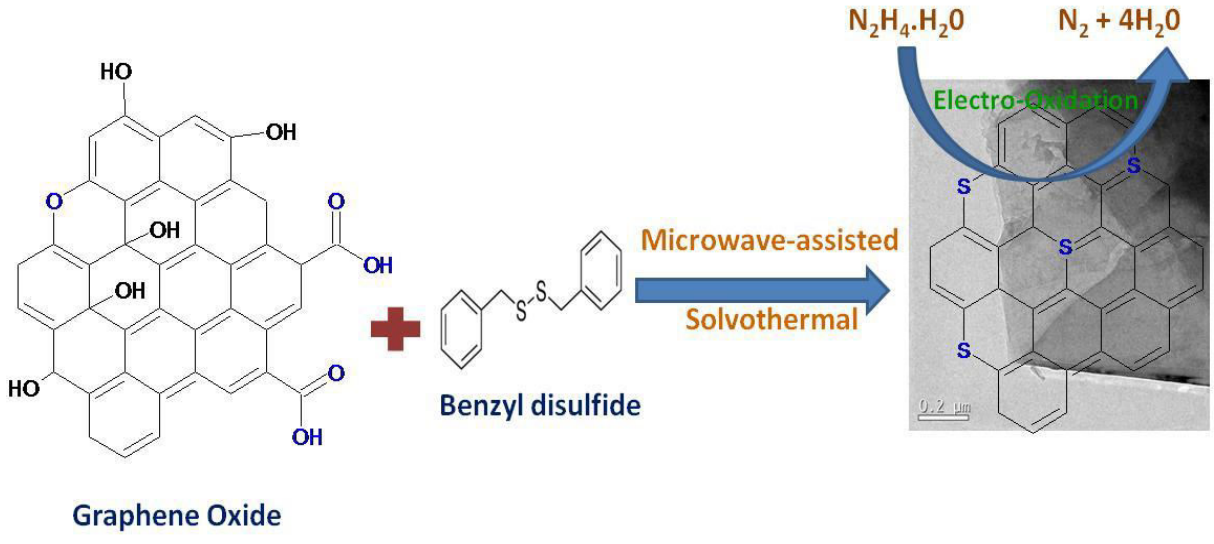
In the present work, binder-free, stable, high-performance and ultrasensitive platform is proposed for the accurate estimation of hydrazine by using a facile synthesized few-layered sulphur-doped graphene (SG)-modified glassy carbon electrode (SG/GCE). This proposed SG/GCE facilitates hydrazine to be catalytically oxidized at low overpotential. The SG was synthesized by a facile microwave-assisted solvothermal route, further examined by electron microscopy, Raman and FTIR spectroscopy and identified as a suitable catalyst material for sensing platform. Experiments were conducted to typify the electrode as a sensor for the estimation of hydrazine. The SG-modified electrode exhibited overpotential of hydrazine oxidation at 0.31 V, which is lower than many other electrochemical sensors. The linear calibration plots were obtained over the range of 0.5–6 µM in chronoamperometry and the limit of detection is as low as 0.25 µM. It is one of the finest reports in terms of high sensitivity and low limit of detection. It is concluded that SG exhibited an efficient sensor platform for hydrazine determination.



Schematic representation of SG synthesis procedure

Keywords: *Sulphur-doped graphene; hydrazine; electrocatalysis; electrochemical sensor; chronoamperometry*

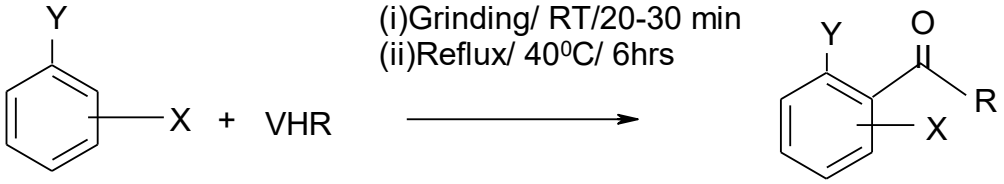
OP:20

Vilsmeier-Haack Formylation And Acetylation Reactions With Phenols Under Solvent Free Conditions

Redamala Roopa

Mahatma Gandhi University

The Vilsmeier-Haack reaction with phenols has been carried out under solvent free conditions. The reactants are taken in a mortar and grounded with a pestle for about 20 to 30 min at room temperature. The reactions afforded formyl derivatives in fairly good yields when a mixture of dimethyl formamide (DMF) and $POCl_3$ is used as VH reagent. However acetyl derivatives were obtained when DMF was replaced by DMA in the composition of VH reagent. Results of solvent free reactions are more superior over solution phase reactions with very good yields and far lesser reaction times. The present finding is more advantageous over solution phase reaction. It is conducted with economically cheap and readily available reagents. The reaction occurs under mild and under environmentally safe conditions with a simple work up at room temperature. Far less reaction times (about 12 times less than thermal reactions) coupled with enhanced reaction yields substantiate that the present work is a major break through in the area of Vilsmeier-Haack synthesis.



Keywords: *Vilsmeier-Haack reaction, phenols, Formyl derivatives, Acetyl derivatives*

OP:21

Synthesis, structural characterization, in vitro DNA binding, and cytotoxic activity properties of Ru(II) compounds containing TMPIP ligand

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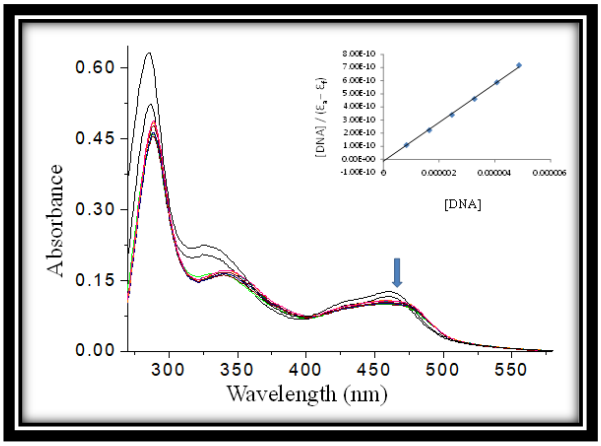
Three ruthenium (II)polypyridyl complexes using 2-(2,4,5-trimethoxyphenyl)-1-H-imidazo[4,5-f][1,10]phenantroline, (TMPIP) as intercalating ligand and phenanthroline, Bipyridine and dimethyl bipyridine asanciliary ligand were synthesized and characterized by using UV-Vis, IR and NMR, Mass spectral methods. These complexes have demonstrated DNA binding ability hence we attempted to study the drug-DNA interactions in detail. Absorption, emission, viscosity titrations were used to investigate the binding of Ru(II) complexes with calf thymus DNA and also investigated photocleavage of plasmid pBR322DNA. Molecular docking studies explored theoretical binding of these complexes. These complexes were assessed for their Antimicrobial and cytotoxic studies.



Key words: *pBR322DNA, calf thymus DNA, cytotoxic, TMPIP, polypyridyl complexes, Absorption, emission, viscosity, photocleavage, anciliary. Intercalating*

OP:22

Synthesis, biological screening and molecular docking of novel imidazole based 1,2,3-triazole hybrids of anticancer and antibacterial activity

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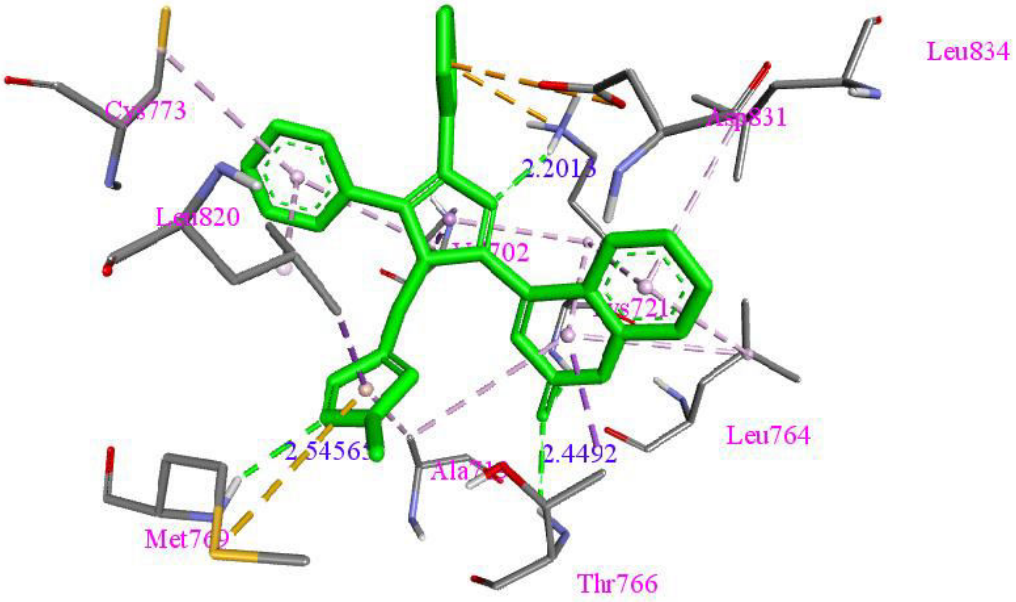
This research represents the synthesis of a novel series of imidazole based triazoles analogues (**5a-o**).All the synthesized compounds were described using ^{1}H NMR, ^{13}C NMR, ESI-mass spectrum and elemental analysis. All these compounds were investigated for their *in vitro* anticancer activity against human cancer cell lines MCF-7, A549 and HeLa by the MTT assay method. The compounds **5d** and **5j** exhibited potent activity against three cancer cells compared with the standard drug cisplatin. The moleculardocking results are well corroborated with the *in vitro* anti-cancer activity finding.In addition, the *in vitro* antibacterial activity of compound **5c** exhibited excellent activity against the microorganisms compared with the standard drug.



Docking interactions of **5d** to the binding sites of target protein EGFR (**PDB ID: 4Hjo**)

OP:23

Design, Synthesis and Biological Evaluation of Amide Derivatives of Thiazolo[5,4-d]pyrimidines as Anticancer Agents.

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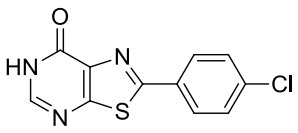
[2.] *Sreenidhi Institute of Science and Technology (Autonomous), Ghatkesar, Hyderabad-501301,Telangana, INDIA*

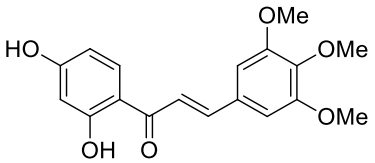
Sulfur and nitrogen hetero-atoms bearing heterocyclic motifs were most significant class of molecules in field of medicinal chemistry.The thiazolo[5,4-d]pyrimidines are a well-recognized fused hetero-aromatic moieties and occupied a prime place in medicinal chemistry. It is considered as an isostere of purine.These displayed a wide variety of biological and pharmacological activities such as CDC25B phosphatase inhibitor,anti-inflammatory, antimicrobial, anticancer, human cytomegalovirus inhibitor, anti-angiogenic, anti-diabetic, neuroprotective,[11]TRPV1 inhibitor,immunosuppressive and phosphatidylinositide 3-kinases. Compound **1** was more potent human adenosine A3 receptor antagonist with hA3AR ki values 18nM.Similarly, α,β-unsaturated framework was found to be one of the most versatile functional group in medicinal chemistry. They were considered as precursor of flavonoids familyand also various types of bioactive molecules.The unsaturated system was found to possess biological activities such as antifungal,inflammatory,tyrosine kinase inhibition, hyperglycaemic, antioxidant, antioncogenic, cardiovascular, antituberclosis, antimalarial, apoptosis, antileishmanial, antimitotic,DNAbinding, anticancer,antibacterial,anti-antiviral,and enzyme inhibition. The (E)-1-(2,4-Dihydroxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one **(2**) has exhibited tubulin binding activity.

Based on the above mentioned biological findings and continuation of efforts, we have designed and synthesized a series of amide derivatives of thiazolo[5,4-d]pyrimidines (**10a-j**). The compounds are evaluated for in vitro anticancer effects against four human cancer cell lines such as PC3 (prostate cancer), A549 (lung cancer), MCF-7 (breast cancer) and DU-145 (prostate cancer) by employing of MTT assay.



2-(4-Chlorophenyl)thiazolo[5,4-*d*]pyrimidin-7(6*H*)-one

(1)



(*E*)-1-(2,4-Dihydroxyphenyl)-3-(3,4,5-trimethoxyphenyl) prop-2-en-1-one

(2)

Figure 1

Keywords: *thiazolo[5,4-d]pyrimidine, in vitro,chalcone, anticancer activity.*

OP:24

Quantitative Estimation Of Residual Solvents In Selected Antiemetics By Headspace Gas Chromatography

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[2]Department of Chemistry, University College for Women, Osmania University, Hyderabad, Telangana State, India.
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Objective:
The presence of residual solvents in pharmaceutical drug substances or products, and excipients may affect the quality and stability of the final product which is highly unacceptable and therefore has to be monitored to ensure its safety and efficacy. The main objective of this study is to develop a Head Space Gas Chromatography (HS-GC) method for the validation and quantitative determination of residual solvents in selected drugs- netupitant API and palonosetron API.

Method: In the developed HS-GC method for the quantitative determination of residual solvents in netupitant API(N-methyl pyrrolidine, xylene, toluene, and N, N Dimethylacetamide) - the headspace equilibrium was achieved at 80℃ which was analyzed using a DB-624column (30m*0.53mm, 3.00µm) with injector and detector temperature set at 160℃ and 230℃ respectively with a total run time of 20mins. For the estimation of residual solvents in palonosetron API(ethanol, acetone, methanol, acetonitrile, and isopropyl alcohol), the headspace equilibrium was formed at 100℃ and analyzed by DB-624 column (30m*0.24mm, 1.8µm)with injector and detector temperature set at 200℃ and 230℃ respectively with a total run time of 20mins. The developed method has been validated and quantified as per International Conference on Harmonization (ICH) guidelines.
Results: All the results obtained were within the ICH specified limits. The validation results for repeatability studies (%RSD values) were found to be less than 10; recovery studies values were in the range of 90-110% and the correlation coefficients(γ^2) for all the solvents were observed to be >0.99.
Conclusion: A sensitive, simple, precise, and economic HS-GC method with Flame Ionization Detector (FID) was developed and validated to quantitatively determine the residual solvents in Netupitant API and Palonosetron API.
Keywords: *Netupitant, Palonosetron, Residual Solvents, Head Space Gas Chromatography,*

OP:25

An Efficient Synthesis of2-Amino 5-Phenyl 1,3,4-Thiadiazole from Phenyl Acetic Acids Via Copper Catalysed Oxidative Decarboxylative Cyclisation

L.Chinnari,B.V.Prasad,L.Rajeswari,Y.Kumari, P.Rajitha Lakshmi and V.Siddaiah*

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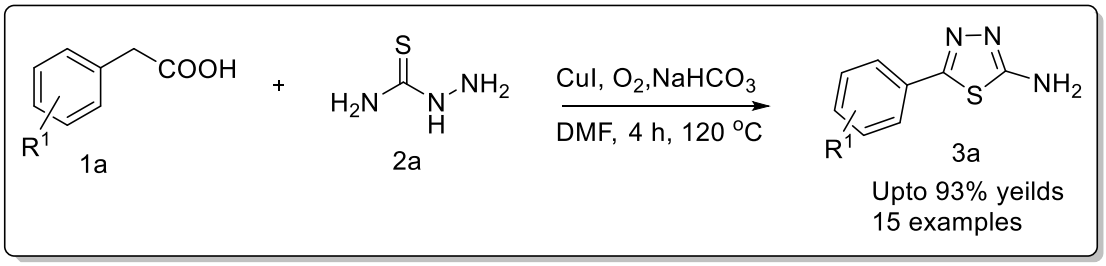
*sidduchem@gmail.com

1,3,4-Thiadiazole derivatives have been elicited interest in medicinal chemistry and agricultural field as herbicides and bactericides.There has been intense investigation of different classes of thiadiazol compounds, many of which possess extensive pharmacological activities. Among them, the compounds which are having 1,3,4-thiadiazole nucleus are known to exhibit biological activities such as antimicrobial,antifungal, antidiabetic, anti-inflammatory, antileishmanial, antituberculosis, anticancer, anti-HIV, antioxidant/ radioprotective, carbonic anhydrase inhibitory activities. Despite their potential applications, only a few approaches are available for the synthesis of 2-Amino 5-Phenyl 1,3,4-thiadiazoles. Generally, these compounds are synthesised by the reaction of thiosemicarbazide with aldehydes or carboxylic acid derivatives.However, these methodshave some limitations as harsh conditions. Therefore, facile and convergent approaches for accessing an array of 2-amino5-phenyl 1,3,4 thiadiazoleare highly desirable. Herein we demonstrate a simple and efficient protocol for the synthesis of 2- amino 5-phenyl 1,3,4-thiadiazoles from Phenyl acetic acids and thiosemicarbazide*Via*Copper catalysed decarboxylative cyclisation in presence of CuI as a catalyst, Oxygen as an oxidant and K_2CO_3 as base at 120 °C for 4h (**Scheme 1**).



Scheme 1: Synthesis of2-Amino5-Phenyl 1,3,4-Oxadiazole

Key words: *Phenyl acetic acid, Copper catalyst, Oxidative decarboxylation, Oxygen atmosphere.*

OP:26

Hatu indused synthesis of n-substituted-1,8-naphthyridinyl benzamide and their biological activity

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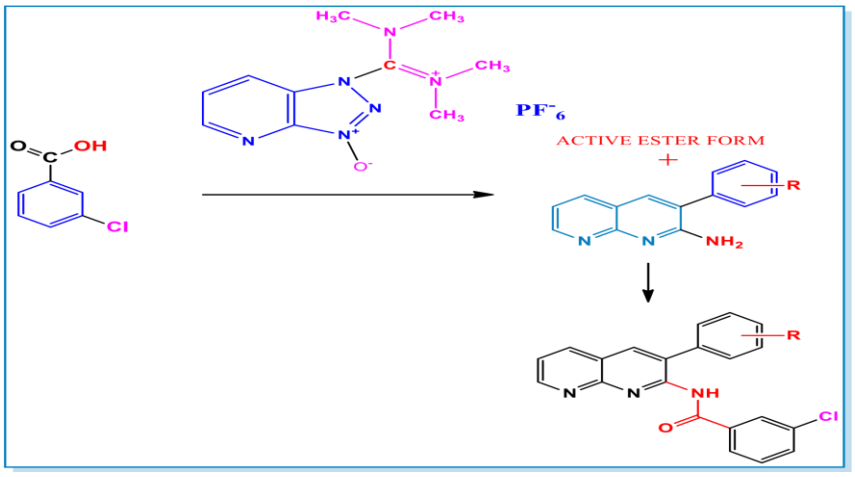
Amide bond construction is a basically very important reaction in organic synthesis Which plays an important role in modern biology.HATU is one of the reagent used in peptide coupling chemistry to generate an active ester form from a carboxylic acid. Aryl benzoic acids which are in presence of HATU gives substituted 1,8-naphthyridin-2-yl-benzamide with substituted 3-phenyl-1,8-naphthyridin-2-aminesat ambient temperature conditions. All newly synthesized compounds were screened for their in-vitro antibacterial activity against grampositive bacteria (Staphylococcus epidermidis) and gram negative bacteria (Escherichia coli). All these compounds exhibited superior activity against the all tested microorganisms.

Keywords: *HATU, Naphthyridin-2-amines,Meta Chlorobenzoic Acid, 1,8-naphthyridin-2-ylbenzamide.*



OP:27

Insilico ADMET Prediction, Synthesis and Biological Evaluation of Nitrogen containing Heterocyclic Compounds

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A series of some novel heterocyclic derivatives were prepared by acetylation of Imidazole and Acetyl chloride to give respective N-acetyl imidazole, which was further reacted with different substituted aromatic aldehydes in the presence of ethanol and NaOH used as base.All the synthesized compounds are confirmed by physicochemical data and spectral analysis ^{1}H NMR, IR and MASS spectra. All the synthesized compounds were predicted using various software's like Molinspiration, Molsoft and OSIRIS. The compounds showed good pharmacokinetic and pharmacodynamics properties. All thecompounds are screened for antibacterial, antifungal and antioxidant activity, the anti-bacterialactivity determined using agar medium by cup plate method. The anti-bacterial activity chalcone derivatives were compared with the standard oflaxacin at concentration of 100µg against two gram positive and two gram negative bacteria, methanol is used as control.The compound 5a, and 5c have significant activity against b.subtilis at conc. 10 and 30 µg/ml.The anti-fungal activity is determined by using potato dextrose agar medium by cup plate method, anti-fungal activity of chalcone derivatives were compared with the standard griseofulvin at concentration of 100µg/mlagainst fungi pencillinium chrysogenum taking methanol as control.The compound 5c has significant activity against pencillium chrysogenum at conc. of 200µg/ml.Anti-oxidant activity is determined by stable free radical method, ascorbic acid is used as the standard, DPPH is used as a control.All the synthesized compounds showed potent antioxidant activity.

Key words: *N- acetyl Imidazole, Osiris, Antifungal activity, DPPH, oflxacin,* **Nutraceuticals vs Pharmaceuticals**

OP:28

Qualitative analysis and antimicrobial activity of the weed *Rivina humilis* (blood berry).

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**Corresponding author: rupasree.ucw@gmail.com*

Terpenoids are the naturally occurring organic chemical compounds that are produced as secondary metabolites in many plant species. Plant extracts of terpenoids have extensively been used for several herbal remedies since ancient times. However, special interest is being shown over utilization of weeds for curing various ailments and diseases. The aim of this preliminary study is to examine the qualitative and quantitative analysis of the weed, *Rivina humilis*(blood berry). The plant has been reported to have some traditional uses in medicine to treat colds, diarrhoea, difficult urination, flatulence, gonorrhea, jaundice and ovarian pain.*Rivina humilis* is a flowering plant, belonging to the *Petiveriaceae* family, (earlier placed in pokeweed family, Phytolaccaceae). The leaves of the plant were collected,dried and plant extract was drawn out by using chloroform as the solvent. Qualitative analysis of phytochemical constituents of the plantextract for terpenoids was carried out and further evaluated for antioxidant activity.The plant extracts were also assessed for their antimicrobial properties to enable their prospective use in herbal medicine.

Keywords: *secondary metabolites, terpenoids, Rivinia humilis, antimicrobial, herbal medicine.*

OP:29

An Efficient Synthesis of2 Amino 5-Phenyl 1,3,4-Thiadiazole from Phenyl Acetic Acids Via Copper Catalysed Oxidative Decarboxylative Cyclisation

L.Chinnari,B.V.Prasad,L.Rajeswari,Y.Kumari, P.Rajitha Lakshmi and V.Siddaiah*

Department of Organic Chemistry & FDW, Andhra University, Visakhapatnam.

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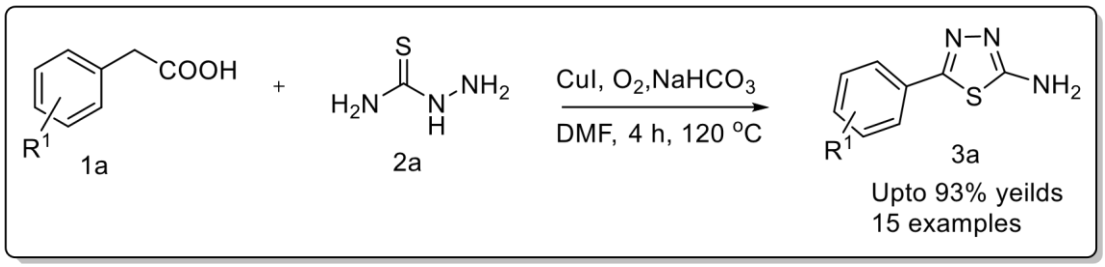
1,3,4-Thiadiazole derivatives have been elicited interest in medicinal chemistry and agricultural field as herbicides and bactericides.There has been intense investigation of different classes of thiadiazol compounds, many of which possess extensive pharmacological activities. Among them, the compounds which are having 1,3,4-thiadiazole nucleus are known to exhibit biological activities such as antimicrobial,antifungal, antidiabetic, antiinflammatory, antileishmanial, antituberculosis, anticancer, anti-HIV, antioxidant/radioprotective, carbonic anhydrase inhibitory activities. Despite their potential applications, only a few approaches are available for the synthesis of 2-Amino 5-Phenyl 1,3,4thiadiazoles.Generally, these compounds are synthesised by the reaction of thiosemicarbazide with aldehydes or carboxylic acid derivatives.However, these methodshave some limitations as harsh conditions. Therefore, facile and convergent approaches for accessing an array of 2- amino5-phenyl 1,3,4 thiadiazoleare highly desirable. Herein we demonstrate a simple and efficient protocol for the synthesis of 2- amino 5-phenyl 1,3,4-thiadiazoles from Phenyl acetic acidsand thiosemicarbazide*Via*Copper catalysed decarboxylative cyclisation in presence of CuI as a catalyst, Oxygen as an oxidant and K_2CO_3 as base at 120 °C for 4h (**Scheme 1**).



Scheme 1: Synthesis of2-Amino5-Phenyl 1,3,4-Oxadiazole

Key words: *Phenyl acetic acid, Copper catalyst, Oxidative decarboxylation, Oxygen atmosphere.*

OP:30

A Facile Synthesis of N,N- dimethyl- 2-substituted -1H-Indole 1-Carboxamides *via* cross dehdrogenative coupling of 2- substituted indoles and formamides.

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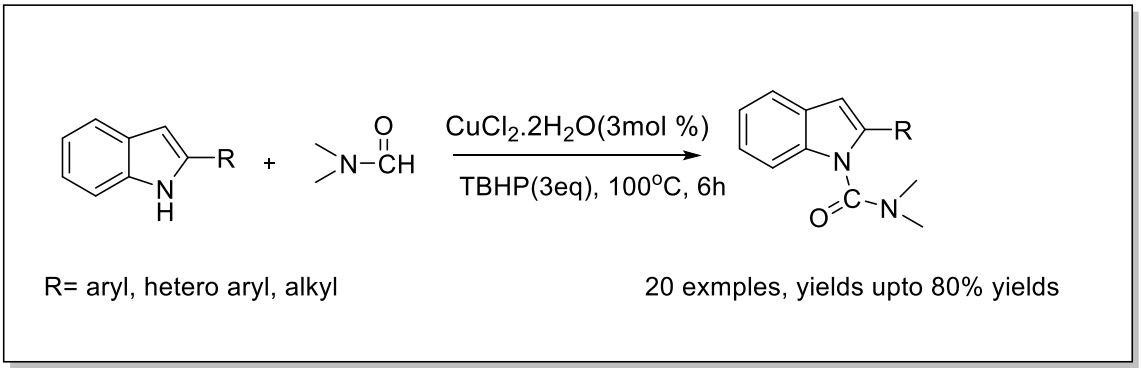
Abstract: Carboxamide derivatives are important heterocycles and recognized as privileged scaffolds due to its various applications in pharmaceutical chemistry and natural products. Heterocyclic moieties having N-Carboxamide group shows a wide range of biological activities like insecticidal, antibacterial anti-proliferative activities. They have also been used as pesticides, for example, indoxacarb is a commercially available pesticide against lepidopteran larvae. On the other hand, Indole ring systems have wide range of pharmacological activities such as antihistaminic, antifungal, antimicrobial, antioxidant, plant growth regulator, anti-HIV, anticonvulsant, anti-inflammatory and analgesic etc. Therefore, it is in high demand to develop new protocol for the construction of 2- substituted indole based N-Carboxamides from easily available starting materials with good yields. So, herein we report a facile method for the synthesis of Indole based N-Carboxamides via formation of C-N bond by cross dehdrogenative coupling of 2- substituted indoles and formamides in the presence of Cu catalyst and TBHP oxidant at 100 ^{0}C temperature for 6 h. In this approach we obtain N, N-dimethyl- 2-substituted -1H-Indole 1-carboxamides in good to excellent yields.

Key words: C-N bond formation, cross dehydrogenative coupling, 2- aryl/alkyl Indole, N, N - dimethyl formamide, carboximide.



Scheme 1: Synthesis of N,N- dimethyl- 2-substituted -1H-Indole 1-Carboxamides

OP:31

Synthesis, Characterization, DNA binding, and Molecular docking studies of Ruthenium(II)polypyridyl complexes

Sravani Gudikandula[1], Aruna Kodipaka[1] and Navaneetha Nambigari[1,2]*

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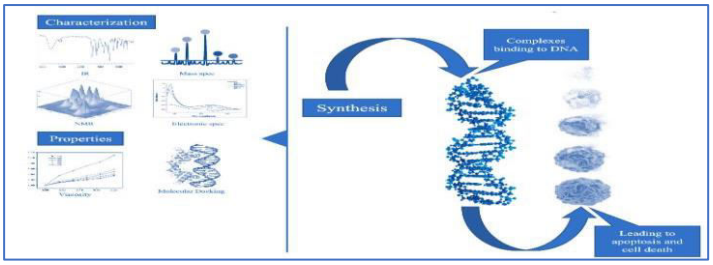
Recent literature on the metal complex interaction with Biomoleculesindicates a significant role in medicine, pharmacy, and diagnostics. Ruthenium-based complexes are known for their impact as drug candidates, though they have very little in common with the existing platinumbased drugs. They are believed to have low toxicity and appreciable selectivity for tumors. The synthesis, choice of intercalator, and ancillary ligand result in interesting spectral profiles, DNA-binding, cleavage, and biological activities.

The present study focuses on the synthesis, characterization, and DNA binding affinity of three Ruthenium (II) polypyridylcomplexes - $[Ru(A)_2QPDA]^{+2}$where A = Ancillary Ligand, (1) phen=1,10-phenanthroline, (2) tbz = 2-(1,3-thiazol-2-yl)-1*H*-benzimidazole,(3) bpy= 2,2' bipyridine, QPDA = Intercalator Ligand, N,N'(8,9 – Quinoxalinedylidene) 1, 10-Phenanathroline – 5, 6- diaminehave been synthesized and characterized. The DNA –binding affinity is investigated by spectroscopic titrations & Mode of binding is assessed by viscosity measurements. The binding constant (K_b) of all the three complexes was determined to be in the order of 1 > 2 > 3. These experimental results showed that all these complexes interact with CT-DNA by intercalative binding mode. The bindingdata of ruthenium complexes was supported by molecular docking studies. The docking analysis reveals that all the complexes bind via intercalation via Guanine-rich regions of DNA.



Key Words: *Intercalator, Ancillary ligand, binding constant, Molecular docking.*

OP:32

Copper - metformin ternary complexes: Thermal, DNA binding and molecular docking studies

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*[2]*Department of Chemistry, Osmania University, Tarnaka, Hyderabad, Telangana State, 500007, India.*

ABSTRACT

Novel three copper(II) complexes of type $[Cu(metf)(o\text{-}phen)_2]Cl_2$ **(1),** $[Cu(metf)(opda)_2]Cl_2$ **(2)**, $[Cu(metf)(2\text{-}2'bipy)_2]Cl_2$ **(3)**, (Metf = metformin, o-phen = ortho-phenanthroline, opda = ortho-phenylenediamine, 2-2' bipy = 2-2' bipyridyl) were synthesized and characterized by various analytical and spectral techniques. The ESR spectra of complexes **1, 2** and **3** measured in DMSO solvent at liquid nitrogen temperature (X-band 77K) and assigned octahedral geometry and metal to ligand bond covalency. The DNA binding properties of these complexes were investigated by absorption, emission and viscosity studies. From the spectral data it was concluded that the complexes bind to DNA through groove mode of binding. The intrinsic binding constants (K_b) from absorption spectroscopy were 10.14×10^4, 1.44×10^4, and 4.05×10^4 M^{-1} for **1**, **2** and **3**, respectively and Stern-Volmer quenching constants (K_{sv}) from emission spectroscopy were 0.30, 1.58, and 0.32, respectively. Thermal degradation pattern of the compounds was studied and Coats-Red fern method is used to determine kinetic parameters for complexes **1**, **2** and **3** from thermal studies. Discovery studio 2.1 software was used to evaluate binding affinity and interaction pattern of complexes with B-DNA receptor protein. C Docker Interaction energy of **1**, **2** and **3** complexes was 30.705, 30.077, and 32.948 respectively, and the highest docking score is seen for complex **3**.

KEYWORDS: *Copper complexes, DNA, docking, groove binding, Metformin.*

OP:33

Pyridine bridged polybenzimidazole for the use in high temperature PEM fuel cell

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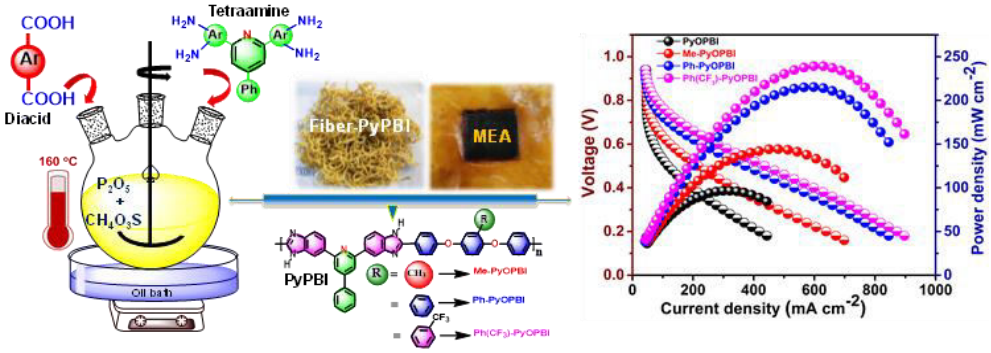
Though pyridine bridged oxypolybenzimidazole (PyOPBI) membranes are considered as the promising high-temperature proton exchange membrane (HT-PEM) material that have the potential to overcome many obstacles *ca.* solubility, membrane processability and cost etc. of the mainstream polybenzimidazole (PBI) based HT-PEM, but the weak structural stability of PyOPBI in Conc.H_3PO_4, poor dimensional stability have been the crucial issues restraining the performance. In order to mitigate these bottlenecks, in this work 3 types of PyOPBIs with flexible backbones were successfully synthesized by polycondensation reaction of various diacids and tetraamine in Eaton's Reagent followed by casting as HT-PEMs. The designed membranes showed considerably high PA loading and proton conductivity (0.04-0.078 S/cm) at 180 °C as compared to earlier reported PyOPBI membranes (0.007 S/cm). In addition, the obtained membranes showcased good chemical, long-term conductivity stabilities and outstanding stability in Conc.H_3PO_4. The pendent groups of the backbone are believed to be the cause behind better stability and facilitating H^+ transport resulting higher proton conductivity. The single cell made from the MEA of these substituted PyOPBI membranes displayed a power density in the range of 144-240 mW cm^{-2} under H_2/O_2 at 160 °C, which is considerably higher than PyOPBI (90.4 mW cm^{-2}). Overall, the current results provide an effective strategy to explore the benefits of structural modulation of PyOPBI using various structurally divergent diacids to enhance HT-PEM properties.



References

[1] Maity, S.; Jana, T. *Macromolecules* **2013**, 46, 6814-6823.

[2] Sannigrahi, A.; Arunbabu, D.; Sankar, R. M.; Jana, T. *Macromolecules* **2007**, 40, 2844-2851.

[3] Yang, J.; David, A.; Li, Q.; Cleemann, N.; Jens Oluf ,J.; Chao, P.; Niels, B. J.; He, R. *ChemSusChem* **2013**, 6, 275-282.

[4] Yang, J.; Li, Q.; Cleemann, N.; Jens Oluf ,J.; Chao, P.; Niels, B. J.; He, R. *Adv. Energy Mater.* **2013**, 3, 622-630.

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OP:34

Zeolite Encapsulated Cu(II),Co(II) Glycine And Histidine Complexes : Synthesis and Characterisation.

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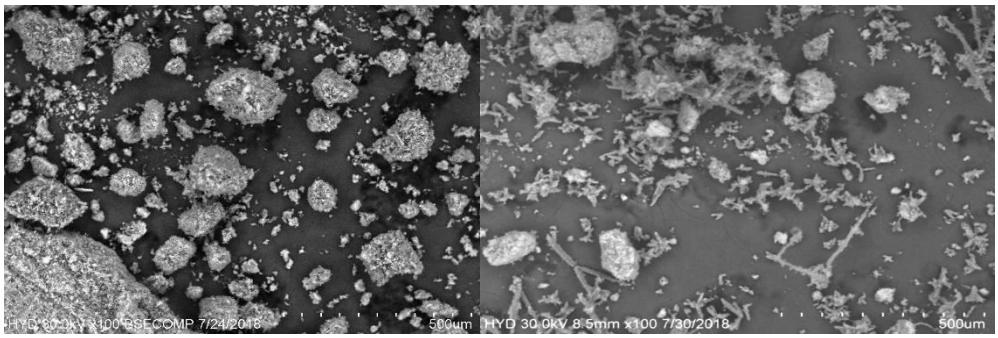
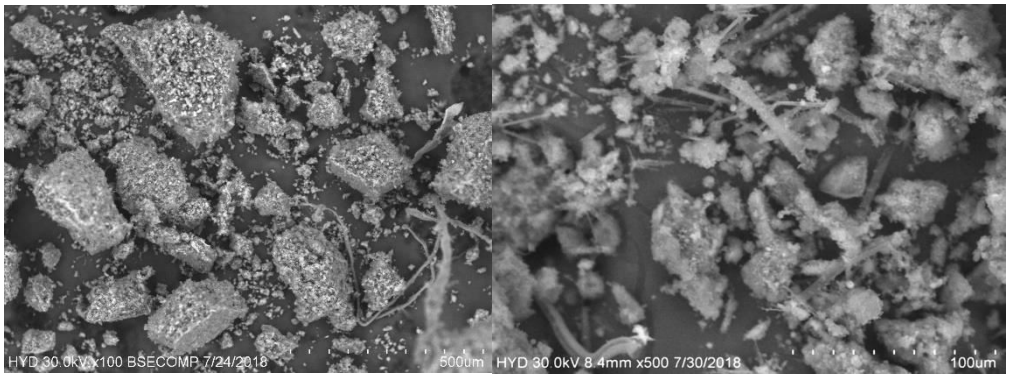
Ternary Cu (II) and Co(II)Complex of Glycine and Histidine is synthesized in situ in Na-Y-Zeolite by the reaction of ion exchanged metal ion with the flexible ligand molecules that had diffused into the cavities. The encapsulated complex is characterised by SEM, XRD, FTIR,UV,ESR, and AAS Spectroscopy. Analysis of data indicates the formation of complexes in the cavities without effecting Zeolite framework structure (XRD).The absence of any extraneous species is obtained from SEM



(A) (B)

Fig1: SEM Micrograms of Gly-Cu(II)-Y-Hist Before(A) And After(B) Soxhlet Ectraction.



(A) (B)

Fig2: SEM Micrograms of Gly-Co(II)-Y-Hist Before(A) And After(B) Soxhlet Ectraction.

Key Words*: Zeolite – encapsulated complex; Na- Y Zeolite, Glycine, L-Histidine, Ion Exchange, Flexible ligand method***.**

OP:35

Use of Hydrogen as a source of clean energy

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Replacement of Hydrogen by a carbon emitting fuel is a best way to get clean environment . It can be of an enormous opportunity to increase business elasticity and decrease the use of fossil fuels that became continuously downscale day by day. Large scale production of "Green Hydrogen " is still a challenging process. In a Fuel Cell, on combination with Oxygen it produces heat and electricity with water – vapour as a side product. In case of Green Hydrogen method, electric current is generated by wind turbine and solar panels through water using an Instrument called "Electrolyser" to split the Hydrogen from water. "Also the concept of Black and Grey Hydrogen" that causes carbon emission." Blue Hydrogen" produced from Coal gasification where carbon- dioxide gets stored beneath the earth crust. "Pink hydrogen" concept also exists, where Nuclear power is used for its creation.

Keywords: *Clean energy, Hdrogen Fossil fuels, Nuclear power*

OP:36

Impact of Clean Energy on Economic Growth: An Empirical Investigation

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The purpose of this paper is to empirically investigate the impact of clean energy, gross capital formation (capital), Labour force (Labour) on Economic growth, particularly in relation to India. The study utilizes annual data from 1990 to 2014. GDP constant prices of 2010 denominated in US Dollar, alternative and nuclear energy (% of total energy use), Gross Fixed Capital Formation (% of GDP) proxy for Capital and Labour force total were obtained from World Bank, World Development Indicators. The study employed descriptive statistics, Correlations, Johansen cointegration test and Pairwise Granger Causality test. Empirical results confirmed the existence of a long-term equilibrium relationship among the variables and showed that clean energy consumption using Granger causality test causes economic growth. We can infer crucial policy implications from the findings. Consumption of clean energy has a favourable impact on economic growth and cuts CO2 emissions significantly. As a result, policymakers should focus on and encourage the development of clean energy.

Keywords: Clean Energy, Economic Growth, Capital, Labour, Correlations, Cointegration Test, Pairwise Granger Causality, India

OP:37

Smart Agroecosystems using Nanosensors

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Agroecosystems are a source of food for mankind. Major challenges faced by agroecosystems include perpetual fluctuating climatic conditions, unceasingly demographic strain, the persistence of lethal heavy metals, and high utilization of resources. To fulfill the food requirements of an ever-growing population, the existing agricultural practices make use of sophisticated machinery, and agrochemicals which have led to an increased level of pollution and deterioration of soil health, thereby affecting human health.

Monitoring of agroecosystems is generally carried out by various methods which include Highperformance liquid chromatography, mass spectroscopy, gas chromatography, etc. But these are high cost, time-consuming, and require skilled personnel. Hence there is an emergent need for quick and economically viable monitoring methods. Nanotechnology has offered rapid development of Nanosensors and biosensors for the detection of contaminants, biological components, and particular molecules. The present paper focuses on various biosensors and nanosensors employed in agroecosystem monitoring and the factors affecting their implementation.

Keywords: *Agroecosystems, challenges, Nanosensors, Biosensors, Factors affecting*.

OP:38

Effect of soil pH on germination and growth of *Triticum aestivum* and *Zea mays*

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Various environmental stresses viz. extreme temperatures, problem soils including soil salinity, drought and flood have affected the production and cultivation of agricultural crops. Among these, problem soil (acidic, alkaline, sodic, and saline) is one of the most devastating environmental stresses, which causes major reductions in cultivated land area, crop productivity and quality caused by variable concentration of ions in the soil. Soil reaction (pH), in particular, is an important variable, perhaps due to its influence on many other soil properties and processes affecting plant growth. Many plant characteristics (i.e., traits) such as height, lateral spread, grains yield, biomass, flower size and number, pollen production, etc., are influenced by the pH of the soil. In this study, we investigated the effects of soil pH on the germination and growth (shoot and root height, yield, dry weight, etc.) of *Triticum aestivum* (bread wheat) and *Zea mays* (corn). Highly acidic soil (pH 4.0) was collected from a site (hotspot) in Sonipat district of Haryana. Simultaneously, problem soils, both acidic and alkaline soils were prepared by fortifying garden soil (pH 7.0) with weak acidic and basic solutions using aluminium sulphate and calcium hydroxide, respectively. Experiments were conducted with replicates, to counter experimental errors. A set of control pots having seeds of wheat and maize grown in garden soil was also set up.

Keywords: *Soil, pH, problem soil, Triticum aestivum, Zea mays*

OP:39

Preparation of biodegradable plastic composites from fruit wastes.

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Organic food wastes have been considered to be a barrier in sustainable development,as their decomposition leads to a tremendous increase in greenhouse gases and creates environmental problems. Similarly, when petroleum-based plastics are used in surplus amounts beyond control, it becomes amajor cause for environmental pollution. In order to overcome these issues and to minimise the plastic and food waste- based problems, biodegradable composites are being prepared as a substitute to these products. Bioplastics are defined as the plastics which are derived from natural resources like fruit waste, biomass, corn-starch, sugarcane and food waste. The bioplastics such as polyhydroxyalkonoates (PHAs) or polyhydroxybutyrates (PHBs) has the ability to replace a number of traditional plastics, which are made up of petrochemicals and serves as potential alternate to the conventional plastic material. These are partially or entirely biodegradable and are relatively less harmful to the environment.

The primary objective of this study is to produce biocomposites from fruit wastes and peels using simple laboratory techniques and to characterize them for various physical and chemical properties. Banana peelsare chosen for the current experiment because of its easy availability and high cellulose content. The polymer produced by using the banana peel using glycerol could help in the formation of a biocomposite having paper-like characteristics with flexibility, pliability,etc. Various laboratoryanalyses like solubility, acid-base sensitivity, and biodegradabilityalong with fourier transform infrared (FTIR) and powder-x-ray diffraction (XRD) analysis would open up avenues for the prospective application of the polymer as a user-friendly biodegradable plastic. These bioplastics can play an important role in the market for sustainable use and can reduce the pollution caused by dumping of plastic and fruit wastes, thereby, providing aneco-friendly alternative.

Keywords: *Bioplastic, sustainable development, cellulose, polyhydroxyalkonoates, polyhydroxybutyrates, biodegradable, eco-friendly.*

OP:40

Mycodiesel - An Alternative and Novel Approach for the Production of Biodiesel

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The diminishing supply of fossil fuels reserves and the environmental concerns have made renewable energy an alternative energy source for the future. Recently, certain fungi are known to produce volatile hydrocarbons which are found similar to diesel. These compounds have potential to be used both as 'green chemicals' and biofuels. The present paper reviews on the *Gliocladium roseum,* one of the first known fungus to be a producer of 'Mycodiesel'.

Gliocadium roseum is a filamentous fungus which is widely distributed in soil and decaying vegetation. It is generally occurring as a saprophyte and never known as a pathogen either in animals or man. *G. roseum* is also act as a biocontrol agent and used in controlling many plant diseases.

G. roseum, produces a series of acetic acid esters of straight-chained alkanes including those of pentyl, hexyl, heptyl, octyl, sec-octyl, and decyl alcohols and some other hydrocarbons such as undecane, 2,6-dimethyl; decane, 3,3,5-trimethyl; cyclohexene, 4-methyl; decane, 3,3,6trimethyl; and undecane, 4,4-dimethyl when grown on an oatmeal-based agar medium and different types of volatile hydrocarbons such as heptane, octane, benzene, and some branched hydrocarbons when grown on cellulose based medium.

It is found that when exposed to threatening substances, the fungus defends itself by emitting volatile gasses. Further, it is also able to convert plant cellulose directly into the biofuel. Crops normally have to be converted to sugar and fermented before they can be turned into useful fuel. So, by utilizing *G. roseum*, it is possible to efficiently cut the extra step in the production of biodiesel. This includes hydrocarbons remarkably similar to those used in diesel engines and therefore they are called as "mycodiesel".

Nearly 430 million tons of plant waste are produced from farmland each year around the world. *G. roseum* provides new hope of turning this green waste into a useful fuel. With its ability to digest cellulose along with the production of volatile hydrocarbons. *G. roseum* make it a potentially exciting new source of biodiesel which can be generated in industrial scale, as a new source of green energy.

Keywords: *Renewable energy, Biofuel, Fungi, Gliocladium roseum, Mycodiesel*

OP:41

Porous activated carbon derived from agro-waste sugarcane pith for enhanced CO_2 capture and MO dye adsorption performance

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In this work, we propose a simple scheme for the synthesis of activated carbon derived from sugar cane pith (SCP-AC). The SCP-AC was characterized in terms of surface area, pore volume, pore diameter, surface morphology, functionalities and structural aspects. The result showed high, selective and stable CO_2 capture performance over N_2using obtained AC. The SCP-AC reached a high adsorption capacity 2.71 mmol/g at 15 ^{0}C under 1 bar pressure. The CO2/N2 selectivity calculated from Henry's law exhibits high adsorption selectivity of 21.41 for CO_2 over N_2 at 15 ^{0}C and 1 bar. Furthermore, in order to better understand the interaction between CO_2 and SCP-AC, the examination ofisosteric heat of adsorption (Q*st*) variesfrom 13.36 to 2.56 kJmol^{-1} has been carried out.The SCP-AC showed the fast removal of MO dye (25 min) with maximum MO adsorption capacity (~527.7 mg/g).Their adsorption behavior including capacity, efficiency, kinetic study, adsorption equilibrium was evaluated using fitting models.

Keywords: *Sugarcane pith (SCP), Activated carbon (AC), CO_2 capture, MO dye removal*

OP:42

Assessment of Water Quality of Major Lakes of Hyderabad

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Our work is focused on assessing the lake water quality parameters like pH, BOD, COD, heavy metal detection, conductivity, TDS, oil and sludge. Thorough our work we have tried to bring focus on deteriorating health of Hyderabad urban lakes due to rapid urbanization.

Key words: *Lake water, quality assessment, Hyderabad*

OP:43

Recovery of Ozone hole

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Ozone, as we know is a chemical made of three Oxygen atoms and exist as a layer 8-30 miles above the earth's surface in the Stratosphere. Chlorofluorocarbons are the main culprits responsible for the depletion of Ozone layer. It is a matter of worrisome for all of us as the depletion of Ozone layer cause harmful UV radiation to reach the earth resulting in damage ranging from crop death to skin cancer. Now, after 33 years, the Ozone layer is showing some signs of recovery. In 2018, it was found that chlorine levels are falling with reduced ozone depletion over Antarctica. Human activities are responsible for the presence of 80 percent of chlorine over Stratosphere. Leakage from refrigerators results in the emission of chlorofluorocarbons'. Currently, the situation of Ozone layer observed is far better than predicted during the period 1990-2010.

Keywords: *ozone, Stratosphere, chloroflurocarbons, UV radiation*

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OP:44

Insilico Spectral and DNA docking studies of Ruthenium (II) polypyridyl complexes.

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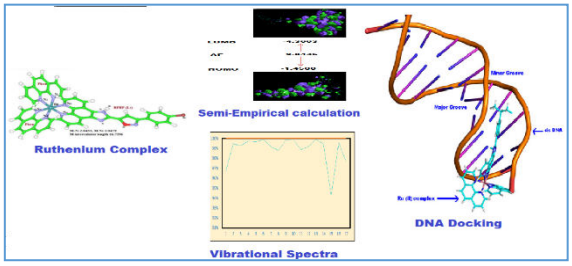
Ruthenium(II) polypyridyl complexes are one of the most extensively studied and developed systems because of their interesting photophysical and photochemical properties. In this viewpoint, explore past and recent works on the spectroscopic, photophysical, and photochemical characteristics of these complexes.

The present study focuses on the Insilico interpretation of vibration spectrum and equilibrium geometries and DNA docking of the [Ru(A)$_2$MTPIP] complexes, where A = Ancillary Ligand, (1) phen=1,10-phenanthroline, (2) dmp = 4,4'- dimethyl phenanthroline, (3) bpy= 2,2' bipyridine, MTPIP = Intercalator Ligand, 2-(4-(methylthio)phenyl)-1H-imidazo[4,5-f][1,10] phenanthroline using the semi-empirical method - PM3. The difference between the observed and calculated wavenumber values of most of the fundamental modes in the molecule is very small. Further, the molecular geometry and electronic properties (Frontier molecular orbital HOMO—LUMO), electrostatic potential surface (ESP) for the complexes was analyzed to give their nucleophilic level of sensitivity. The ESP is a useful property to study reactivity given that an approaching electrophile will be attracted to negative regions (where the electron distribution effect is dominant). The significance of ESP lies in the fact that it is very useful in the research of molecular structure with its physiochemical property relationship. The stabilities of the complexes were obtained from the quantum chemical parameters, calculated using the HOMO - LUMO energies. Additional parameters such as HOMO - LUMO energy gap, absolute hardness, and absolute softness are calculated. The Ru (II) complex - DNA docking study reveals that the Ru(II) polypyridyl complexes bind to DNA preponderantly by intercalation. The results show that the phen and dmp complex has a more effective binding ability than the bpy, indicating the role of the ancillary ligand in determining their specificity for DNA binding.



Keywords: *Photophysical, Vibrational spectrum, Frontier molecular orbitals, DNA Docking, Polypyridyl ligands.*

OP:45

Ensemble Pharmacophore Meets Molecular Docking: A Novel Screening Approach for the identification of β-Tubulin Inhibitors.

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The major component of microtubules i.e, β-tubulin is considered as an attractive molecular target of several small molecules for treatment of cancers. In the present research, various computational studies were performed to develop prognostic 3D-QSAR models using a series of Dithiocarbamate derivatives as β-tubulin inhibitors for anticancer activity. Using 90 inhibitor molecules having PIC50 in the range of 4.012 to 8.141 a pharmacophore model was built up. For proper alignment of all inhibitor molecules a five-point common pharmacophore model was generated using a training set of 47 and test set of 43 molecules using PLS Factor 3.

The generated pharmacophoric hypothesis AAHRR.1 (two hydrogen bond acceptors, one hydrophobic group and two aromatic rings) has excellent values of R2=0.955, Q2=0.616, F=304.2, Pearson R=0.7864, RMSE=0.5058. Then virtual screening was performed by using Asinex Elite Synergy, Otava databases and identified several hits. Then the molecules which had crucial interactions with β-tubulin were obtained by performing SP & XP dockings for obtained hits. The molecular docking studies of these inhibitors at the binding pocket of β-tubulin showed vital interactions with Leu 252, Val 238, Asp 251, Asn 258, Val 315, Cys 241, Tyr 202 amino acids. We have also designed 14 new Dithiocarbamate inhibitors. Almost 11 molecules exhibited crucial ligand interactions and docking scores more than the standard. The above findings led us in identifying new molecules with β-tubulin inhibitor activity, which could be used further to design molecules with better pharmacokinetic properties.

Key words: *β-tubulin, Molecular Docking, Pharmacophore model, Virtual screening, ADME Properties, Dithiocarbamate derivatives.*

OP:46 2D QSAR and molecular docking studies on Iso-Combretastatin derivatives as Microtubulin complex inhibitors

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Cancer is an ever-growing public health situation affecting millions of people every passing year. Development has been gradually witnessed with respect to both the cancer treatment and the perception of people towards cancer. New drugs, treatment procedures and prevention methods are taking cancer treatment to a whole greater level. One of the important targets for cancer is the Microtubulin complex. Herein we report a 2D QSAR and docking studies on series of Iso-Combretastatin derivatives as Microtubulin complex inhibitors. Molecular docking and SAR like 2D QSAR, ADME studies were performed to design a chemical entity. The developed 2D QSAR model had an excellent R (correlation coefficient) value of 0.905 and R^2 Pred (cross validation coefficient) value of 0.744. The outcomes of this study give us an insight for designing novel and peculiar Microtubulin inhibitors and provides us with the guidelines for designing compounds with improved Novel inhibitory potential.

Key words: *Cancer, Microtubulin, IsoCombretastatin, CADD, ADME, QSAR, Molecular Docking*

OP:47

Unfolding the 3d Structure of the KSK2 Protein and Identifying Novel Scaffolds against it: a Paradigm for discovering new Tb Therapeutics.

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Tuberculosis is a contagious disease caused by the bacteria *Mycobacterium tuberculosis*, and it is one of the leading causes of death every year. Prolonged therapeutic regimens, multi-drug resistant tuberculosis, recurring tuberculosis, and socioeconomic conditions are all factors contributing to the upsurge of tuberculosis. The COVID-19 pandemic has increased the rate of infection in infected people, necessitating the development of innovative therapeutic lead compounds against potential tuberculosis drug targets (Global tuberculosis report 2021).KSK2 is a nucleotide-binding domain of the trehalose transporter complex that facilitates trehalose absorption from host cells, which assists in growth, survival, and virulence. As a result, the prediction of three-dimensional structure and identification of novel scaffolds against the KSK2 protein aids in the discovery of new medications to contribute to the TB therapy pipeline. To generate the 3D model of KSK2 protein, template proteins from *Mycobacterium smegmatis* with PDB IDs 7CAD-C and 7CAG-C were selected by applying template search methods.Multiple sequence alignment of the target protein and experimental templates were used to predict the 3D structure of the KSK2 protein with Modeller 9.10v. The predicted structure reliability was assessed by several validation techniques, and a putative binding pocket was found using the CASTp webserver. The findings were compared to the KSK2 protein binding site (37-G,38-P,39-S,40-G,41-C,42-G,43-K,44-T,45-T,83-Q). Energy minimization, protein-protein docking, protein-liganddocking, and virtual screening experiments were carried out using the Schrodinger suite modules and online server tools. The data were analyzed for new scaffolds based on docking score and docking energy parameters.

KEYWORDS: *Mycobacterium tuberculosis, Virtual screening, Homology Modelling, Active site prediction.*

OP:48

QSAR Studies on HIV-1 Protease inhibitors -A Battle against HIV using Computational Chemistry

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HIV/AIDS is a major public health problem. Despite the advances in HIV treatment, the cure for all HIV patients still possesses a major challenge, which needs to be surpassed in coming years. One attractive target is HIV-1 Protease. Herein we report a new series of HIV-1 Protease Inhibitors incorporating stereo chemically defined tetrahydrofuran-tertiary amine-acetamide P2 ligand. Structure activity relationship studies like 2D QSAR, ADME studies and Molecular Docking were performed to design a chemical entity. A total of 37 compounds were chosen for this study divided into Training and Test set. A total of 27 training set molecules were taken for the SAR analysis (2D QSAR). The model was seen to have an incredible Correlation coefficient (R=0.942) and also exhibited good predictive power confirmed by the high value of cross validated correlation coefficient (Q^2 = 0.701). The outcome of this study gives us an insight for designing novel and peculiar HIV-1 Protease Inhibitors and provides us a guideline for designing compounds with improved HIV virus inhibitory potential.

Keywords: *HIV-1, Protease Inhibitors, QSAR, Molecular Docking*

OP:49

Identification of New Lead Molecules against SWM Protein for Cancer Therapy.

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Glioblastoma (GBM) is one of the most aggressive types of cancer that begins in the brain and is challenging to treat. The newly diagnosed patients with GBM usually undergo the surgical resection of the tumor followed by radiotherapy. However, radiotherapy is the preferred treatment given to every patient with GBM at an early stage. But the GBM cells are highly resistant to radiation. As a result, the tumors are not permanently eradicated. Therefore, increasing the sensitivity of GBM cells to radiation is a promising approach for improving the survival of GBM patients. Previous studies deduce that SWM protein knockdown will increase the GBM cells to radiation. Hence, it becomes important to inhibit SWM protein to increase the sensitivity of GBM cells to radiation. The present studies include in silico methods to identify the inhibitors for SWM protein. To analyze the binding interactions of SWM protein with the lead molecules, the 3D structure was generated using homology modeling and validated using standard computational techniques. The active site of the SWM protein was predicted usingCASTp, FTServer, and GalaxyWeb server tools. The binding region of SWM protein was considered for the docking study. Virtual screening of phytochemicals from Indian medicinal plants was selected as ligands for docking studies to generate small ligand inhibitor structures. The prioritized ligands with acceptable ADME properties are reported as new lead molecules against SWM protein for GBM radiosensitization treatment.

KEYWORDS: *Glioblastoma, Radiotherapy, Radiosensitization, In silico methods, Lead Molecules*

OP:50

Investigation on benzothiazole-imidazole derived Schiff base: Reconnoitring from DFT Studies

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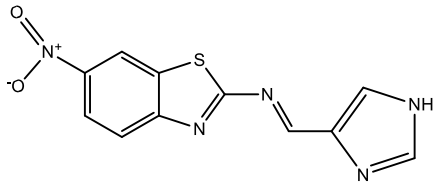
Computational chemistry acts as emerging trend data repositories for the discovery of novel materials. Inorder to construct a new material, need to understand the phenomena influencing the properties of materials and undertaking activity at the atomic level. Electronic properties of materials explore the basic physical principles that underlie charge and excitation transport assists the designing of materials. Density Functional Theory (DFT) marks a decisive breakthrough in solving electronic structure for the description of the ground and excited states of organic materials. DFT, a theoretical description of hundreds of electrons, generally predicts the ground state geometries, vibrational spectra, UV-Vis spectra, HOMO-LUMO energy levels, atomic charge distribution and natural bonding orbitals to explore the inter and intramolecular interactions. Herein, we report a new benzothiazole derived Schiff base ligand, (E)N-((1H-imidazol-4-yl)methylene)-6-nitrobenzo[d]thiazol-2-amine, was geometrically optimised using B3LYP/6-311++G (d,p) levels of theory and characterised by theoretical electronic, vibrational and NMR spectra. The other properties such as, Frontier Molecular Orbitals, Molecular electrostatic potential, Mulliken charge analysis and global reactivity parameters etc. were also analysed. Though benzothiazole moiety was well known for its biological activity, Molecular docking simulation was also carried out to explore the protein (BSA) binding interaction.



Keywords: *Schiff base, DFT Studies, HOMO-LUMO, MEP, Mulliken, Molecular docking.*

OP:51

Molecular Modelling and Phase Studies For Identifying Novel PI3K/AKT/MTOR Inhibitors

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The serine/threonine kinase AKT is a key component of the PI3K/AKT/mTOR signalling pathway as it exerts a pivotal role in cell growth, proliferation, survival, and metabolism.In order to find out novel Akt1 inhibitors which have different scaffolds, pharmacophore-based virtual screening, molecular docking, and binding free energy were calculated. A five-point pharmacophore hypothesis with two hydrogen bond acceptor (A), one hydrogen bond donor (D), and two aromatic rings (R) was developed with acceptable R^2 and Q^2 values of 0.93 and 0.67 respectively. Then by using Asinex Elite Synergy database, virtual screening was performed, and identified several potential hits. Subsequently, the molecules which had interactions with the target akt1 were determined by subjecting the obtained hits for SP and XP docking processes. Finally, for the top leads obtained, binding free energies were accomplished. Some new molecules were also designed. Almost 10 molecules manifested crucial ligand interactions and binding free energies. At the outset, this research paved the way for us in spotting new molecules with AKT1 inhibitory activity, which can further be explored to design molecules with enhanced pharmacokinetic profiles.

References

1) Siu T, Liang J, Arruda J, et al. Discovery of potent and cell-active allosteric dual Akt 1 and 2 inhibitors. BIOORG MED CHEM LET. 2008; 18: 4186-4190.
2) Scheid MP, Woodgett JR. Unravelling the activation mechanisms of protein kinase B/Akt. FEBS LETT. 2003; 546: 108-112.
3) Cheng JQ, Lindsley CW, Cheng GZ, et al. The Akt/PKB pathway: molecular target for cancer drug discovery. Oncogene. 2005; 24: 7482-7492.

OP:52

CONVENTIONAL AND GREEN SYNTHESIS OF AZOMETHINE DERIVATIVES OF BIOLOGICALLY IMPORTANT ALDEHYDES

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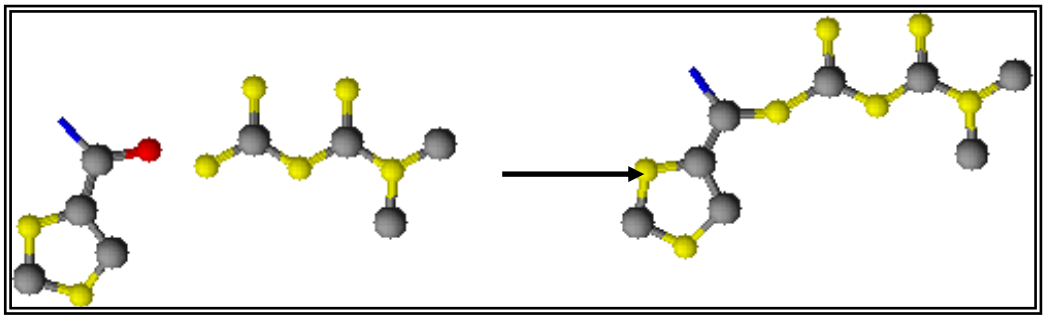
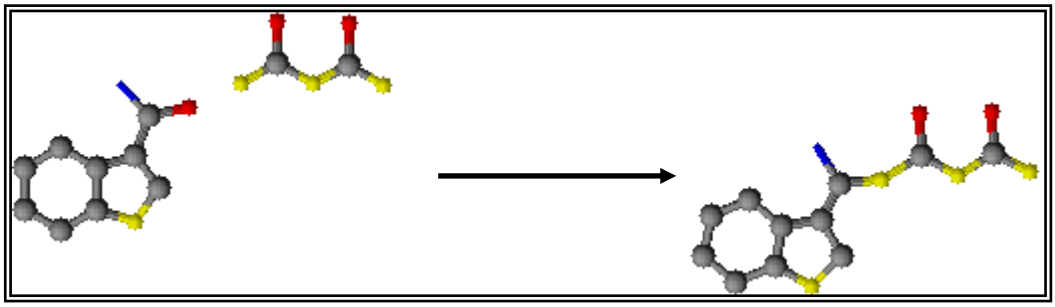
ABSTRACT

The chemistry of azomethine (-CH=N-R') compounds is an important area of research with increasing interest due to the simple synthetic protocols, their versatility, and diverse ranges of applications. The presence of functionalized carbocyclic and/or heterocyclic moieties of aromatic and non-aromatic skeletons has been shown to be a promising pharmacological strategy to enhance the biological activity of azomethine compounds. To alleviate critical environmental concerns with organic synthesis, Green Chemistry has gained tremendous impetus, as it promotes chemical products and processes that mitigate and/or eliminate the use and generation of hazardous materials. Some biologically important aldehydes and primary amines of important grade have been selected for the synthesis of azomethine skeletons in conventional as well as microwave methods in the presence of natural acids like citric acid. The compounds under study were subjected to spectral analysis for structural elucidation. The synthesized compounds have been used for the evaluation of applications, biological activity, DNA binding studies, and anti-oxidant activity. Further, they are also incorporated for the fabrication of metal-organic frameworks (MOF) to study the applications based on intrinsic information present in its structure.

Keywords: Azomethine, Green synthesis, characterization, and biological activity studies





OP:53

GREEN SYNTHESIS OF COPPER NANOPARTICLES USING AQUEOUS ALTERNANTERA SESSILIS (Linn.) LEAF EXTRACT AND THE STUDY OF ANTIOXIDANT, PHOTO CATALYTIC AND ANTIBACTERIAL STUDY

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ABSTRACT

In the present study, phyto-fabricated Copper nanoparticles (CuNPs) were prepared from aqueousleaf extract of *Alternanthera sessilis* by a facile, economic, and eco-friendly approach. The facile phytofabrication of CuNPs was confirmed by UV-visible spectroscopy with characteristic peak around λmax of **560-570nm**, FTIR spectroscopic analysis and Zetapotential analysis confirmed that *TC*-Cu NPs were synthesized by phytoconstituents of *Alternanthera sessilis*aqueous leaf extract, negative charge (-29.1 mV) reveled the formation stable Alternanthera sessilis-Cu NPs. The XRD pattern showed that synthesized *Alternanthera sessilis*-Cu NPs were crystalline in nature with FCC structure. The SEM images depicted that *Alternanthera sessilis*-Cu NPs were irregular in shape. The spherical shape and size of about 3-12 nm were revealed by TEM analysis. The biogenic Cu NPs demonstrated fascinating dose dependent antioxidant activity with EC50% as 68.73g/ml, and highest activity as 58.36 at 100 g/ml, as well as significant Photo catalytic activity against Congo red dye, which was completely degraded after 20 minutes. Furthermore, the studies revealed that Cu NPs displayed greater antibacterial efficacy against Gram negative bacteria than Gram positive bacteria.

Key Words: *Alternanthera sessilis*, Metabolites, Biosynthesis, Copper Nanoparticls, Antioxidant.

ABSTRACTS OF FULL PAPERS

FP:01

Qualitative analysis and antimicrobial activity of the weed *Rivina humilis* (blood berry).

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Terpenoids are the naturally occurring organic chemical compounds that are produced as secondary metabolites in many plant species. Plant extracts of terpenoids have extensively been used for several herbal remedies since ancient times. However, special interest is being shown over utilization of weeds for curing various ailments and diseases. The aim of this preliminary study is to examine the qualitative and quantitative analysis of the weed, *Rivina humilis*(blood berry). The plant has been reported to have some traditional uses in medicine to treat colds, diarrhoea, difficult urination, flatulence, gonorrhea, jaundice and ovarian pain.*Rivina humilis* is a flowering plant, belonging to the *Petiveriaceae* family, (earlier placed in pokeweed family, Phytolaccaceae). The leaves of the plant were collected,dried and plant extract was drawn out by using chloroform as the solvent. Qualitative analysis of phytochemical constituents of the plantextract for terpenoids was carried out and further evaluated for antioxidant activity.The plant extracts were also assessed for their antimicrobial properties to enable their prospective use in herbal medicine.

Keywords: *secondary metabolites, terpenoids, Rivinia humilis, antimicrobial, herbal medicine.*

FP:02

Protective Effects of Turmeric Against Cisplatin Induced genotoxicity on bone marrow cells of mice

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The inorganic platinum compound cisplatin (CP), has been used as a cancer therapy for decades and exhibits strong anti-tumor activity. However, the wide application of Cisplatin is largely limited due to its side effects. Natural therapies, such as the use of plant-derived products in cancer treatment, may reduce adverse side effects. In the present investigation studied the possible anti genotoxicity effects of Turmeric ethanolic extract on chromosomal aberrations induced by Cisplatin in the bone marrow cells of mice.The results indicate that Turmeric extract decreased significantly the percentage of chromosomal aberrations induced by Cisplatin in a dose dependent manner indicates the anti genotoxic effects of Turmeric.

Key Words: *Cisplatin, Turmeric, Antigenotoxicity, Chromosomal Aberrations, Bone Marrow*

FP:03

Synthesis of Sulfur Doped Graphene and its Electrocatalytic Application for Hydrazine Determination

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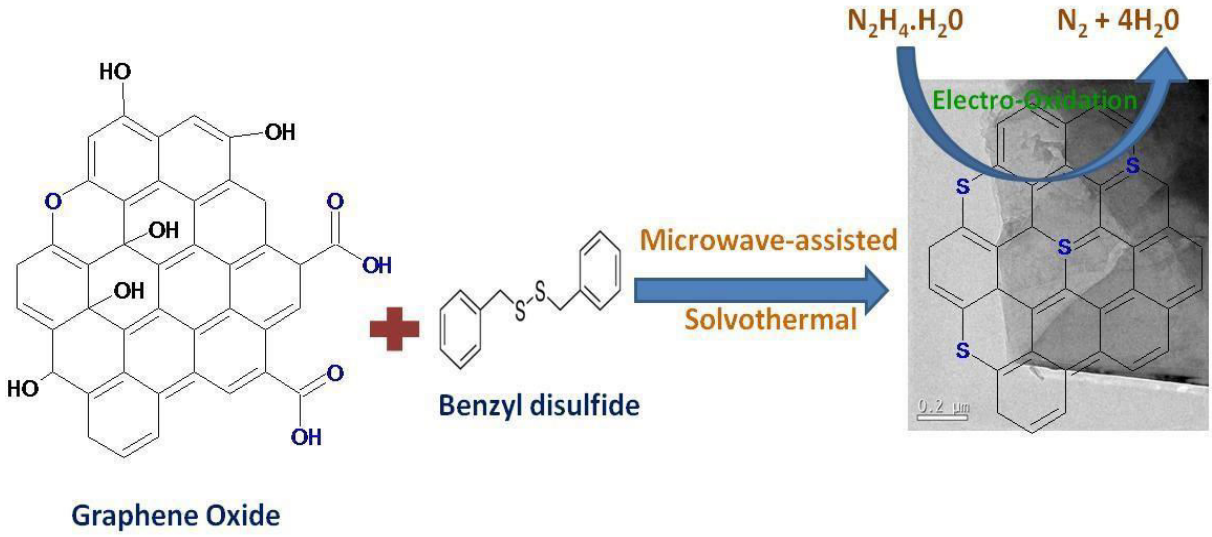
In the present work, binder-free, stable, high-performance and ultrasensitive platform is proposed for the accurate estimation of hydrazine by using a facile synthesized few-layered sulphur-doped graphene (SG)-modified glassy carbon electrode (SG/GCE). This proposed SG/GCE facilitates hydrazine to be catalytically oxidized at low overpotential. The SG was synthesized by a facile microwave-assisted solvothermal route, further examined by electron microscopy, Raman and FTIR spectroscopy and identified as a suitable catalyst material for sensing platform. Experiments were conducted to typify the electrode as a sensor for the estimation of hydrazine. The SG-modified electrode exhibited overpotential of hydrazine oxidation at 0.31 V, which is lower than many other electrochemical sensors. The linear calibration plots were obtained over the range of 0.5–6 µM in chronoamperometry and the limit of detection is as low as 0.25 µM. It is one of the finest reports in terms of high sensitivity and low limit of detection. It is concluded that SG exhibited an efficient sensor platform for hydrazine determination.



Schematic representation of SG synthesis procedure

Keywords: *Sulphur-doped graphene; hydrazine; electrocatalysis; electrochemical sensor; chronoamperometry*

FP:04

Use of Hydrogen as a source of clean energy

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Replacement of Hydrogen by a carbon emitting fuel is a best way to get clean environment . It can be of an enormous opportunity to increase business elasticity and decrease the use of fossil fuels that became continuously downscale day by day. Large scale production of "Green Hydrogen " is still a challenging process. In a Fuel Cell, on combination with Oxygen it produces heat and electricity with water – vapour as a side product. In case of Green Hydrogen method, electric current is generated by wind turbine and solar panels through water using an Instrument called "Electrolyser" to split the Hydrogen from water. "Also the concept of Black and Grey Hydrogen" that causes carbon emission ."Blue Hydrogen" produced from Coal gasification where carbon- dioxide gets stored beneath the earth crust. "Pink hydrogen" concept also exists, where Nuclear power is used for its creation.

Keywords: *Clean energy, Hydrogen Fossil fuels , Nuclear power*

FP:05

Smart Agroecosystems using Nanosensors

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Agroecosystems are a source of food for mankind. Major challenges faced by agroecosystems include perpetual fluctuating climatic conditions, unceasingly demographic strain, the persistence of lethal heavy metals, and high utilization of resources. To fulfill the food requirements of an ever-growing population, the existing agricultural practices make use of sophisticated machinery, and agrochemicals which have led to an increased level of pollution and deterioration of soil health, thereby affecting human health.

Monitoring of agroecosystems is generally carried out by various methods which include High performance liquid chromatography, mass spectroscopy, gas chromatography, etc. But these are high cost, time-consuming, and require skilled personnel. Hence there is an emergent need for quick and economically viable monitoring methods. Nanotechnology has offered rapid development of Nanosensors and biosensors for the detection of contaminants, biological components, and particular molecules. The present paper focuses on various biosensors and nanosensors employed in agroecosystem monitoring and the factors affecting their implementation.

Keywords: *Agroecosystems, challenges, Nanosensors, Biosensors, Factors affecting*.

FP:06

Ascaridia galli (chicken nematode) as a source for Nanoparticle and Nanofiber

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Green synthesis of nano particles and nanofiber gained relevance in recent times. Ideally nanoparticles and nanofiber are made from metallic sources. However, in recent times, there are reports of drastic side effects about the use of metallic nanoparticles in biology and medicine. In this context, it has become more relevant to explore and identify, more natural and biofriendly and effective alternative to metallic ones. There are instances, where, nano particles and nanofibers, and many other nano components, have been synthesized from more natural sources, such as bacteria, different species of algae and also from fungi. However, not many have attempted to synthesize nanoparticles, from unusual sources such as nematodes, the intestinal parasites of animals and humans. For the first time, in the present study it was attempted to synthesize nanoparticles and nanofiber from the intestinal nematode of chicken, *Ascaridia galli*. The parasites, were extracted and isolated from the chicken intestines, they were later processed for the synthesis of nanoparticle and nanofiber. It is quite evident that nanoparticles, synthesized from a natural source are more appealing as they are both eco friendly and inexpensive. Parasite, measuring approximately 30-80mm in length were carefully removed from chicken intestines and later processed for the synthesis of nano particle and nano fiber. Nanoparticles were synthesized using the method of acid hydrolysis and nanofiber was prepared using electro spinning technique. The nanofibre which was synthesized, was hydrophilic in nature, and measured about 6cm x 3cm in size. Scanning electron microscope (SEM)images of nanoparticle revealed a diameter of 48.46nm- 20µm and the nanofiber diameter was found to be between 88nm-2 µm, thus matching to the average standard size of nano particle and nanofiber. As the intestinal parasites, are capable of evading host immunity and can easily amalgamate with the host tissues, without triggering any antagonism, therefore can be used frequently in biology and medicine. As these nanoparticles and nanofiber, are synthesized using a parasite,(a living source) it can easily be degraded after the use, and may be considered as a suitable alternative to metallic nanomaterials.

Key words: *Nanoparticle , nanofiber, Ascaridia galli. electro spinning, SEM, chicken nematode*

FP:08

Synthesis and Characterization of Nanoparticles Heterocyclic Compounds

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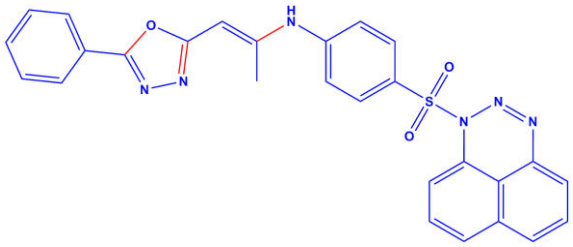
Abstract

The reaction between 4-((1H-naphtho[1,8-de][1,2,3]triazin-1-yl)sulfonyl)-N-(4-(hydraziny loxy)-4-oxobut-2-en-2-yl)aniline and benzaldehyde in the presence of iodine yielded novel heterocyclic compound,4-((1H-naphtho[1,8-de][1,2,3]triazin-1-yl)sulfonyl)-N-(1-(5-phenyl-1,3,4-oxadiazol-2-yl)prop-1-en-2-yl)aniline (NTOD). The novel synthesized compound was characterized by spectroscopic method. In aqueous media novel synthesized heterocyclic compound NTOD's nanoparticles prepared by re-precipitation method. These nanoparticles characterized by using UV-Vis spectrophotometer and scanning electron microscope (SEM). SEM shows the size of the nanoparticles were around 70-100 nm. There is head to head alignment (J aggregate) of the molecules of NTOD during the aggregation which was confirmed by the maximum of absorption spectrum of the dispersed nanoparticles is red shifted by 5 nm from the molecular absorption spectra of the NTOD in the solution.



Keywords: Heterocyclic compound, Nanoparticles,Oxadiazoles, Prparation, spectroscopic data analysis.

FP:09

Ensemble Pharmacophore Meets Molecular Docking: A Novel Screening Approach for the identification of β-Tubulin Inhibitors.

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Abstract:

The major component of microtubules i.e, β-tubulin is considered as an attractive molecular target of several small molecules for treatment of cancers. In the present research, various computational studies were performed to develop prognostic 3D-QSAR models using a series of Dithiocarbamate derivatives as β-tubulin inhibitors for anticancer activity. Using 90 inhibitor molecules having PIC_{50} in the range of 4.012 to 8.141 a pharmacophore model was built up. For proper alignment of all inhibitor molecules a five-point common pharmacophore model was generated using a training set of 47 and test set of 43 molecules using PLS Factor 3. The generated pharmacophoric hypothesis AAHRR.1 (two hydrogen bond acceptors, one hydrophobic group and two aromatic rings) has excellent values of R^2=0.955, Q^2=0.616, F=304.2, Pearson R=0.7864, RMSE=0.5058. Then virtual screening was performed by using Asinex Elite Synergy, Otava databases and identified several hits. Then the molecules which had crucial interactions with β-tubulin were obtained by performing SP & XP dockings for obtained hits. The molecular docking studies of these inhibitors at the binding pocket of β-tubulin showed vital interactions with Leu 252, Val 238, Asp 251, Asn 258, Val 315, Cys 241, Tyr 202 amino acids. We have also designed 14 new Purinylpyridine Dithiocarbamate inhibitors. Almost 11 molecules exhibited crucial ligand interactions and higher docking scores compared to the standard. These findings led us in identifying new molecules with β-tubulin inhibitor activity, which could be used further to design molecules with better pharmacokinetic properties.

Key words: β-tubulin, Molecular Docking, Pharmacophore model, Virtual screening, ADME Properties, Dithiocarbamate derivatives.

REPORT

DEPARTMENT OF CHEMISTRY
UNIVERSITY COLLEGE FOR WOMEN, Koti, Hyderabad-095

Two Days Virtual International Conference on "**Chemical Advances for Sustainable Development (CASD 2022)"**

Dates: 12th and 13th April 2022

Day-1 12th April 2022, Tuesday

The inaugural session began with the welcoming of Guests by **Mrs. M. Sravanthi**, Asst. Professor, Department of Chemistry, UCW. It was followed by the significance of the Conference explained by **Dr. G. Vijaya Lakshmi**, I/c Head and Convener, Department of Chemistry, UCW suggesting that the chemical sciences have the potential to provide solutions for the world's challenges in the future. Hence, nature of the chemistry research needs to be more diverse, inclusive, sustainable and environmentally benign. **Prof. M. Vijjulatha** madam, Principal, UCW has addressed the participants on this occasion and has congratulated the Department of Chemistry for their excellent efforts in organizing the International Conference and selection of speakers for the Conference which finds its relevance in today's world. Guest of Honour **Prof. U. Umesh Kumar garu**, Head, Department of Chemistry, University College for Science, Osmania University, Hyderabad while applauding the Organizing committee for conducting the International Conference, has indicated that the conference is focussing on the globally relevant issues and recent developments. Chief Guest **Prof. Battu Satyanarayana garu**, Hon'ble Vice-Chancellor, Karnataka Central University, Karnataka has opined that such Conferences need to be conducted to focus on key environmental issues such as wastage of chemicals, chemical pollution, industrial pollution, etc and has to be addressed for sustainable and safe future of the world. Keynote Speaker was introduced by Dr. K. Premalatha, Asst. Professor, Dept. of Chemistry UCW. Keynote speaker **Prof. Govardhan Mehta**, Professor, FRS University Distinguished Professor & Dr. Kallam Anji Reddy Chair, has presented an inspiring and informative lecture on the topic "Chemistry – A pivotal science for sustainability of people and the planet". Sir opined that chemistry can give solutions for clean and green environments, solvent less chemistry, etc. Sir focussed on circular chemistry – zero waste chemistry, three Rs, C2C chemical design, chemistry involvement as growth engine, two wake up calls, renaissance of ammonia synthesis for sustainability, pitching for humility, etc. The inaugural session with formal vote of thanks.

Invited Lecture – I

Session Coordinator – **Dr. A. Swaroopa Rani**, Assistant Professor, Department of Chemistry, UCW

Speaker: Prof. P. V. Anantha Lakshmi, Professor, Department of Chemistry, University College for Science, Osmania University, Hyderabad

Prof. P. V. Anantha Lakshmi madam has presented lecture on the topic "Thermogravimetric Analysis – kinetic and thermodynamic parameters" and explained about thermal analysis, thermogravimetric analysis, TG and DIG curves, Coats and Redfern methods, different experimental methods in TG experiments, different models to calculate R2, applications related to thermal stability and graphical and data analysis of various parameters related to TGA.

Invited Lecture – II

Session Coordinator – **Dr. P. Mamtha**, Assistant Professor, Department of Chemistry, UCW
Speaker - Dr. B. Beeraiah, Associate Professor, Department of Chemistry, IIT Madras, Chennai.

Dr. Beeraiah Sir spoke on the topic "Bronsted acid Catalyzed Domino reactions for rapid generation of polycyclic systems". Sir explained about the development of new synthetic methodologies using alkynes and propargylic alcohols as building blocks. Sir focussed on Domino reactions which involves C-C and C-X bond forming transformations under the same reaction conditions. He applied the Domino approach for the synthesis of polycyclic spirocyclic and natural products which are of biologically importance. Also, Sir explained about Meyer Schuster rearrangement reactions which is very novel and highly informative.

Invited Lecture – III

Session Coordinator – **Dr. Aliya Begum**, Assistant Professor, Department of Chemistry, UCW

Speaker: Dr. Raghu Chitta, Department of Chemistry, NIT, Warangal, Telangana

Dr. Raghu Chitta has delivered an informative talk on "Borondipyrromethene based fluorescent chemosensors" formed by involving organic Donor-Acceptor diads through linkers and electron transfer reactions. He has meticulously explained about the investigation of sensing mechanism, fluorescent enhancement studies and computations studies. He also explained about the applications of various spectro-analytical studies employed for the characterization of organic sensors as well highlighted about the detection of hypochlorite using harpic.

Invited Lecture – IV

Session Coordinator – **Dr. N. Kavitha**, Assistant Professor, Department of Chemistry, UCW

Speaker - Prof. Ajay Kumar Mishra, Professor, Department of Chemistry, School of Applied Science, Kalinga Institute of Industrial Technology (KIIT) Deemed University, Bhubaneswar, Odisha.

Prof. Ajay Kumar Mishra delivered lecture on the topic "Nano-engineered composite materials for Environmental sustainability". Sir explained about environment safety and water pollution which is a major concern and needs to be solved on urgent basis. Sir has focussed on how do stain resistant materials work, how do electronics keep getting smaller & is it possible for Cancer patients not to have side effects. He has emphasised on possible methods of preparing nanoparticles – Top down Vs bottom up approaches. Sir also spoke about future uses and possibilities of Nanoscale materials - optical engineering, defence, Security, Bio-engineering, Cosmetics, Nano-fabrics, medicines and drugs. Sir explained about synthesis of nano Composite materials - polymer composites for heavy metal uptake using adsorption techniques, Akron water Supply treatment process - graphical method, polymer clay nanocomposite for waste water treatmenta by Adsorption of contaminants, polymer clay nano composite – microinjection, moulding, scanning electron micrographs & polypyrole glycine doped ironoxide nanocomposite usage for Cr(VI) removal by magnetic separation. To increase reusabilly of used green nanomaterial, to convert lab scale into pilot scale operations, to develop commercially viable, high sustainbility material and how to increase awareness among young scientists.

Technical Session – I 2.15 PM – 4.30 PM

Technical sessions were conducted in parallel mode with Groups A and B:

Group A - As a part of Two day virtual International Conference on chemical Advances for Sustainable Development, Technical session -I for oral presentation was started at 2.15 pm on 12th April 2022. Out of 16 participants alloted under Group A, 10 participants presented their research work in powerpoint from various universities like Osmania, Kakatiya, Andhra university. Oral presentations were evaluated by **Dr. A. Hari Padmasri**, Associate professor, Department of Chemistry, UCS, Osmania university and I/c Head & Convener Dr. G. Vijaya Lakshmi, Department of Chemistry, UCW was also present. Technical session for Group-A was coordinated Dr. Ravi Kiran and Mrs. J. Sowmya, Dept. of Chemistry, UCW.

Group B: Oral presentations for the Group B parallel Technical Session was evaluated by **Dr. M. Kavitha**, Assistant professor, Department of Chemistry, UCS, Osmania University along with Convener **Dr. V Shashikala**, Department of Chemistry, UCW. In this group, 16 presenters have presented their research work in excellent and precise manner in the stipulated

period of time. Evaluators have participated actively by giving necessary suggestions to the participants and encouraging them. Overall, the technical sessions on first day went on well without any technical any glitches. Technical sessions was coordinated by Dr. L.Yamini and Mrs. P. Revathi, from Dept. of Chemistry, UCW.

Day-2 13th April 2022, Wednesday

Invited Lecture – V

Session Coordinator – **Dr. S. Sreekanth**, Assistant Professor, Department of Chemistry, UCW

Dr. G. Sudhakar Reddy, Smart Solutions USA Inc., University of Michigan Sustainable Coordinator.

Speaker gave an informative talk on Green Chemistry leading to Sustainability Development in the learning and teaching methods". Sir explained the concept of green chemistry and sustainability. He then enlightened on 12 Green Chemistry principles with real time examples. He also gave real world examples where green and sustainable development are used like PLA cups, biodegradable bioplastics that degrade into fertilizer, ozone laundry, usage of green chemical for textile and automotive industry. The main highlight of the talk was jpw teachers can implement greener chemical experiments for the undergraduate labs like usage of microscale chemicals and apparatus, minimizing water wastage, energy conservation by using microwave methods. He also informed us of various reference books and journals that are useful for students to learn about green chemistry methods.

Invited Lecture – VI

Session Coordinator – **Dr. M. Neelamma**, Assistant Professor, Department of Chemistry, UCW

Dr. Addepalli Balasubramaniam, Rieveschl Laboratories for Mass Spectrometry, Department of Chemistry, University of Cincinnati, Cincinnati.

Topic – Mass spectrometry-based detection of post translational modifications in proteins. Sir explained about his research work and about disulphide bond detection and xenobiotic isasperlite detection by deamination and dehydration. Sir explained the applications of MS in molecular weight determination, identification and quantification, impurity analysis and structure determination. Explained about usage of different types of detectors and mass analyzers used in MS and its applications in chemistry, environmental testing, food testing, pharma and biopharma testing, LC – tandem mass spectrometry

Invited Lecture – VII

Session Coordinator – **Dr. Ch. Sudhakar Reddy**, Assistant Professor, Department of Chemistry, UCW

Dr. Radhakishan Motukuri, Senior Chemical Engineer / Material Scientist, Pacific Northwest National Laboratory, Richland, Washington, US.

Sir delivered lecture on the topic "Engineered nanoporous materials for potential applications for energy and environment". Sir explained about PFAS research, sources of PFAS like coating on brushes, etc. harmful role of PFAS to health, explained about fluorocarbon interactions in nanoporous materials, current strategies for PFAS remediation as sensors, in capture and destruction. Successful detection of TeO4- in ground water by sensor technique, developing and testing engineered nanoporous materials for targeted PFAS treatment in tap water. Sir explained that PNNL is engaged in sensor commercialization efforts based on the existing patent approach.

Invited Lecture – VIII

Session Coordinator – **Dr. K. Ashwini**, Assistant Professor, Department of Chemistry, UCW

Dr. Jayanthy Subbalakshmi, Associate Professor, BITS Pilani, Hyderabad Campus, Telangana

Madam delivered a lecture on Molecular materials based on organic donor pi acceptors and polymers. She explained about various aspects of molecular materials such as their uniqueness, their applications and fabrication of these materials into optical, electronic and optoelectrical devices. Later on, the Residue switching memory device applications were described wherein the fabrication and methodology was explained. Solar cell application was discussed along with TCNQ derivatives which show fluorescence and anticancer activity. Polymers which are various form of polyelectrolyte templated polyanilines were briefly discussed. The talk was very much apt to the theme of the conference on sustainable development as the materials are water soluble and easily degradable.

Session Coordinator – **Mrs. J. Sowmya**, Assistant Professor, Department of Chemistry, UCW

Prof. D. Basavaiah, Professor, School of Chemistry, University of Hyderabad, Hyderabad.

Sir delivered the talk on the topic "Baylis-Hilman reaction – our recent contribution". Sir exemplified the significance of two component and three component Baylis-Hilman reactions and applications of Baylis-Hilman adducts. Sir explained about the philosophy of research as "How we think is more important than wwhat is actually present".

On the second day of International Conference, in Group D, 14 oral presentations were presented by the participants from various universities across the country. Session Coordinators **Mrs. Ameena Hussain** and **Mrs. Narmada** have well-coordinated with the participants and Evaluator for the session **Prof. K. Girija Mangathayaru**, Professor, Department of Chemistry, Palamuru University, Telangana state have given several useful suggestions to the participants and interacted with them. In Group C, Evaluator **Prof. G. Vijaya Charan**, Professor, Department of Chemistry, UCS, Osmania University, have actively interacted with the participants from various parts of the country, gave them informative suggestions and judged them from their presentations and a total of 14 presenters have shared their research work in the technical sessions. Technical Session Coordinators **Dr. E. Srivalli and Dr. Ayub Shaik** have well coordinated the technical sessions and conducted smoothly.

The valedictory session was conducted on 13th April 2022 at 4.00 PM. The guests were welcomed by **Mrs. M. Vijayatha**, Asst. Professor, Dept. of Chemistry, UCW. Convener and I/c Head, Department of Chemistry, UCW **Dr. G. Vijaya Lakshmi** has presented report on the Two Days Virtual International Conference. The Honorable Vice-Chancellor of Osmania University **Prof. D. Ravinder Sir** and OSD to VC Sir **Prof. B. Reddya Naik Sir** have graced the occasion and congratulated the organizers for the conduct of the Conference on a theme which is apt for the present day challenges faced globally and expressed need for more such kind of academic programs in the future as well. Guest of Honour **Prof. D. Ashok Sir**, BSR Fellow and Emeritus Professor, Department of Chemistry, UCS, OU in his message, said that the theme of the Conference is very important currently and have invited eminent speakers in this field from across the world. Conferences are needed to exchange the ideas with eminent speakers, can learn many new things from the deliberations, gain knowledge in the theme and get new and novel ideas for sustainable research. Sir gave several examples for sustainable energy resources and the role played by chemistry in sustainable growth. Industry-Academia interaction also plays a very important role for achievement of objectives related to sustainability. Sir have extensively spoke about the harmful effects of tobacco, usage of plastics, etc and steps to mitigate it. **Prof. M. Vijjulatha**, Principal, UCW opined that the conference gains importance during the time when UN also insists on Sustainable Development and how Green Chemistry plays an important role in today's scenario. As many speakers of the Conference have also reiterated the same by citing several examples related to environment, sustainability and saving the earth, madam suggested that one should focus on issues pertaining to sustainability too. **Vice-Principal Dr. B. Shailaja** madam congratulated the Department of Chemistry, UCW for coming up with the International Conference on Chemical Advances for Sustainable Development, the theme related to sustainable development goals and on the much needed issues to discuss. Madam applauded that Department of chemistry always conducts the academic programs systematically and

successfully. The valedictory session ended with a formal vote of thanks by Convener **Dr. V Shashikala**, Department of Chemistry, UCW.

Mrs. J. Annapurna, Asst. Professor, Dept. of Chemistry, UCW and **Mr. Hari Prasad**, Exam Branch, UCW have rendered Technical support to the program. **Mrs. G. Sravani** took care of the Feedback form. Various **Committee Members** have given their support and cooperation for the successful conduction of the Conference.

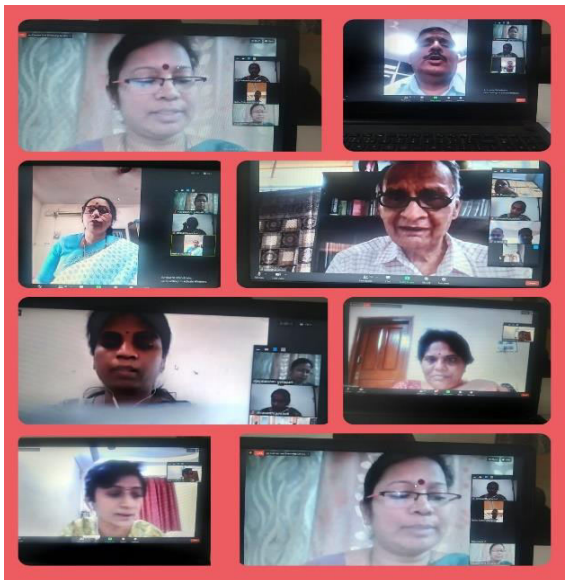
Towards the end of the Valedictory Session, the cash prizes were announced for the best presentations of the Technical Sessions held on both days of the Conference. The presenters who won cash prizes are as follows:

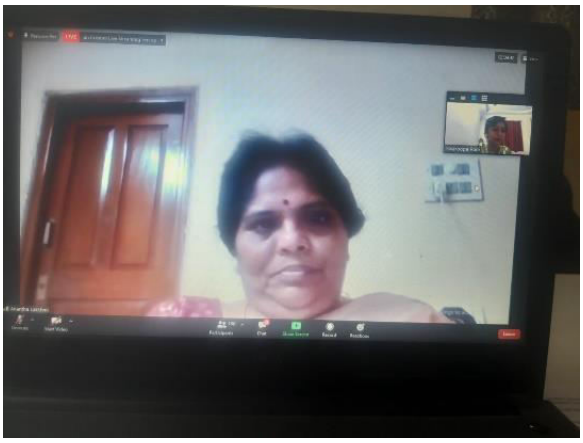
1. Mr. A. Ramesh & group, University College for Women, Koti, Hyderabad.
2. Mr. K. M. Garedkar & Group, Shivaji University, Maharashtra
3. Ms. Rajanandini Kashyap & Group, CSIR-IICT, Hyderabad
4. Ms. Pooja Bajaj & Group, CSIR-IICT, Hyderabad

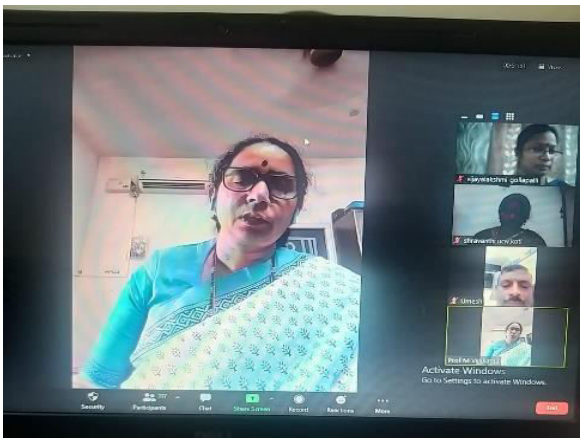
The Brochure for the Two Days Virtual International Conference on Chemical Advances for Sustainable Development (CASD-2022) was formally released in the Principal's Office on 28th February 2022 and the Google form link was open for registrations. The participation for the conference was requested in various forms such as participation, oral presentation, abstract and full paper contributions. Till the last date of registration i.e., 7th April 2020 at 5.00 PM, when the registrations were closed, 220 registrations, 104 abstracts, 90 oral presentations and 25 full papers have been received. The participants were from various states such as Jammu and Kashmir, Madhya Pradesh, Maharashtra, Andhra Pradesh, Delhi, Tamilnadu, Gujarat, Uttarpradesh, Karnataka, Haryana besides Telangana have participated. Abstracts were received from countries like Dubai, UAE, North Eastern Africa, different parts of US and Oman. Abstracts were from various universities, Degree Colleges and premier institutions like CSIR-IICT, APS University, Rewa, Palamuru University, Telangana, University of Nizwa, University of Hyderabad, RGUKT, Basar, Andhra University, Andhra Pradesh, MGU University, Telangana, Kakatiya University, Telangana, Sushant University, Satavahana University, University of Delhi, Manonmaniam Sundaranar University, Tirunelveli, Indian Bureau of Mines, Nizam College, OU, Saifabad PG College, OU, Jaysinghpur college, Jaisinghpur, RBVRR women's college, TSWRAFPDCW Bhongir, Mai-Nefhi College of Science, Asmara, Eritrea, GDC Basholi, Vellore Institute of Technology, Vellore, etc to name a few.

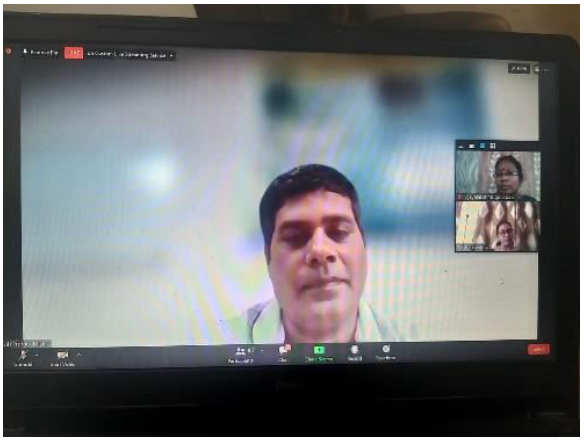
PHOTOS

Day – 1 12th April 2022









Day – 2 13th April 2022