ISBN-ACSSD-2021
9 788192 362885

Vidya Prasarak Mandal’s

B. N. BANDODKAR COLLEGE OF SCIENCE (AUTONOMOUS) THANE, INDIA

NAAC re-accredited 'A' grade

Proceeding of

the National Online Conference on

Advances in Chemical Sciences and Sustainable Development (ACSSD-2021)

April 9 & 10, 2021

Organized by

Department of Chemistry
Vidya Prasarak Mandal’s
B. N. Bandodkar College of Science (Autonomous) Thane, India.

In collaboration with

HBSU

Department of Chemistry,
The Institute of Science
Dr. Homi Bhabha State University, Mumbai,
India.

Vision : Imparting quality education in science

Mission : To mould students into rational thinkers, competent workers and socially aware citizens

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ISO 9001:2015; Best College Award, (University of Mumbai)
"Milestone Merit Leadership" Award; Ramkrishna Bajaj National Quality Award
Recipient of FIST "O" Level
Recipient of grant for STAR College scheme (DBT)
College with Potential for Excellence (CPE) from UGC
Dhyanadweep, Chendani Bunder Road, Thane, Maharashtra 400601

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Published by:
Department of Chemistry
VPM's B. N. Bandodkar College of Science (Autonomous) Jnanadweepa",
Chendani Bunder Road, Thane (W) 400601,
Maharashtra,
India. Tel: 022-25336507
www.vpmthane.org

Citation: Proceedings of the National Online Conference on Advances in Chemical Sciences and Sustainable Development (ACSSD-2021) Edited by Dr. A. S. Goswami- Giri, Dr. S. S. Kahandal, Mr. N. R. Gulvi, Published by Department of Chemistry, V.P.M.'s B. N. Bandodkar College of Science, (Autonomous) Thane 400601; April, 2021.

BEST COMPLIMENTS FROM PATRON

Hon.DR.V.V. BEDEKAR, CHAIRMAN, VIDYA PRASARAK MANDAL

Message from desk of the
Convener in Chief & I/C Principal

I am happy to present this volume of proceedings of the National Conference on Advances in Chemical Sciences and Sustainable Development (ACSSD 2021) and extend my best wishes for the National Conference. Chemistry and advances therein have always been leading progress in modern human civilizations for the past few centuries.

VPM's B. N. Bandodkar of Science (Autonomous), with constant guidance, support and blessings of Vidya Prasarak Mandal, Thane has been on the forefront and always been very proactive in taking on such initiatives. The National Conference jointly organized by our B. N. Bandodkar College of Science (Autonomous) and the Institute of Science, Dr. Homi Bhabha State University, Mumbai is one further step in this qualitative venture which has a legacy of over twenty years in our Jnanadweep campus. I congratulate the Departments of Chemistry of both collaborating institutions.

Here I take the opportunity to recognize and appreciate the efforts taken by the grass root workers, student members and organizing team members from Departments of Chemistry of both institutions who have been working tirelessly for the past several months for successful organization and conduct of this national conference and this volume of its proceedings.

With Best Wishes for success of the National Conference

Capt. Dr. Moses J. Kolet
I/C Principal
VPM's B.N. Bandodkar College of Science (Autonomous)
Thane

Director's Message

It gives me immense pleasure that Department of Chemistry, The Institute of Science has organized a two-day National Conference on "Advances in Chemical Sciences and Sustainable Development" in collaboration with VPM's B.N. Bandodkar College of Science.

The Institute has carved a niche in the annals of instruction since its inception in 1920 by Lord Sydenham and has successfully completed hundred years of quality education. The Institute has lifted a lion's share of Mumbai University in imparting advanced education in all branches of sciences and has also trained students in research. The Institute was chosen for Potential for Excellence by the University Grant Commission (UGC) and has been reaccredited with A grade by the National Assessment and Accreditation Council of India (NAAC).

The Institute has been very fortunate to have in its years a number of brilliant teachers and researchers in the chemistry viz. Dr J. Fox, A N Meldrum, Dr. T S Wheeler, Dr. J R Merchant, Prof. BC Haldar, Prof. Darshane, Prof. Shinde and Prof. Salunkhe and many more.

In recent past, the Institute has been instrumental in furthering the establishment of the Dr. Home Bhabha State University. The Department of Chemistry boasts of 160 students by papers and more than 50 students working for their doctoral degrees. The performance of the students at the University examination has always been outstanding every year. The research students are contributing immensely for the wealth of scientific knowledge by their discoveries in the various fields. The area of research includes nanomaterials, organic syntheses, drugs discovery, computational chemistry, environmental chemistry and analytical chemistry. The department is equipped with modern sophisticated instruments and is also trying for the post-doctoral fellowship.

I wish grand success to the participants of the conference.

Dr. Jairam M. Khobragade
Director, The Institute of Science,
Dr. Homi Bhaba State University, Mumbai

Convener's message

I am extremely happy and pleased to organize and convene the National Conference "Advances in Chemical Sciences and Sustainable Development" [ACSSD-2021 (Online)] in the joint collaboration between Department of Chemistry VPM's B.N. Bandodkar College of Science (Autonomous) Thane and Dr. Homi Baba State University, The Institute of Science, Mumbai. We are thankful to HBSU for their collaboration. This conference is held online due to prevailing corona pandemic situation.

As the Convener of the conference, I welcome and extend my warm greetings and regards to all the delegates' resource persons, participants, students, researchers and volunteers.

The main objective of the National Conference is to bring together academician's researchers and experts from industry. Conference will provide them opportunity and much needed platform to exchange views and acquire ideas, knowledge and latest information and to make them build right kind of opinion. It will help Synthesize hypothesis w.r.t. Latest developmental aspects, concepts and advanced techniques, technology in chemical sciences and its related branches. Student participants are expected to be enriched, empowered and excelled in terms of awareness and competence to face modern day challenges.

We all are proud and privileged to be part of VPM's B.N. Bandodkar College of Science (Autonomous) Thane was established in 1969 by great visionary and educationist Dr. V.N. Bedekar to cater and fulfil the educational needs of the young minds in and around Thane region. Star awarded Chemistry Department is mainly catering to the needs of students who wants to pursue undergraduate and post graduate and Ph.D.

We all are extremely thankful to our patron Dr. V. V. Bedekar, Chairman Vidya Prasarak Mandal Thane. The college has now achieved excellence and grown into educational hub, epicenter of knowledge and wisdom.

We are also thankful to our Ex. colleagues Dr. S.M Sarang, S.G. Madhekar, V.S. Barkule, Mrs. M.P. Akolkar, Dr. A.N. Bedekar, Dr. M.V. Rathnam for their contributions in development of Chemistry department.

We are all thankful to our college I/C principal Dr. Moses Kolet for his support and guidance and Dr. Jairam M. Khobragade, Director Institute of Science, Mumbai. Dr. Mrs. Gayatri Barbade, Joint Convener of the Conference and both the Co-Conveners Dr. Mrs. Anita Goswami-Giri and Dr. Mrs. Sushma Ambadekar and all other members of organizing committees for extending their valuable help in organizing the Conference and also the authors, reviewers of research papers/poster presenters for their active participation.

Dr. D. R. Ambavadekar

Convener’s message

Science is a way of thinking much more than it is a body of knowledge. – Carl Sagan

I am glad to host this Conference on “Advances in Chemical Science and Sustainable Development” in collaboration with VPM’s B.N. Bandodkar College of Science and welcome all the participants. The conference aims to bridge the researchers working in academia and other professionals through research presentations and keynote addresses.

I thank the Principal of Bandodkar College, Dr. Moses Kolte for the opportunity to conduct this event, Also, would like to thank Dr. Anita Goswami Convener Bandodkar College. I thank my colleagues Dr. Bangde, Dr. Banewar and Mrs. Vilhekar extending their invaluable time in organizing the program and all the authors, reviewers, and other contributors for their sparkling efforts and their belief in the excellence of Department of Chemistry of the Institute.

Dr. Gayatri Barabde

Co-convenor's Message

Dear Delegates,

With great pleasure and pride, we welcome you all to the virtual National Conference, On "Advances in Chemical Sciences and Sustainable Development" (ACSSD-2021)

India has inherent qualities for new findings which is evident from well-known narrations. Therefore, we are keen to inculcate the habit of logical thinking in research to enhance their potential as researcher. Our institute and its leadership believe in "Our brain which has a capacity for learning that is virtually limitless which makes every human a potential genius." Hence, it strives for promotion of research culture by organizing two workshops before the any conferences where students put forth their ideas. It will be a good forum to explore various avenues for research in chemical sciences.

The main motive of the conference, to inculcate scientific temperament among young buddies because it brings all the researchers, practitioners from academia and industries towards common goal of advances in chemical sciences for sustainable development.

This would not have been possible without the confidence instilled by our Dr. V. V. Bedekar, Chairman Vidya Prasarak Mandal and the innovative direction of our Principal and Chief Convener of the conference Capt. (Dr.) Moses Kolet. Also, this was possible due to encouragement of Dr. D. R. Ambavadekar, Vice Principal, Head of the chemistry Department and Convener of the conference who is retiring in the month of May-2021.The second workshop was dedicated to the Ambawadekarsir. The contribution of all organizing committee and national advisory committee has given strength and support for this conference. Special thanks to student volunteers for their arranging technical program.

We feel honoured for the collaboration with Department of Chemistry, Dr. Homi Bhabha State University, Institute of Science, Mumbai and are Thankful Dr. Khobragade , Dr. Malaghe and Dr. Gayatri Barabde, for collaboration and cooperation throughout this journey.

Our sincere thanks are due, to all our eminent Chief Guest, Keynote & invited speaker, reviewers and Technical Program Committee members and all participants. With this Once again welcome you all.

"Chemistry states the more energy you put into a bond the harder it is to break"

Thank you once again!

Dr. Anita S Goswami-Giri
Associate Professor in Chemistry,
VPM's B. N. Bandodkar College of Science
(AUTONOMOUS), Thane (W)-1

Dr. Sushama Raju Ambadekar
Associate Professor in chemistry
The Institute of Science,
Dr. Homi Bhabha State University,
Mumbai

Organizing Secretaries' Address

We would like to extend a warm welcome to all delegates to the National Conference on Advances in Chemical Sciences and Sustainable Development (ACSSD-2021), which is being organised by the Department of Chemistry, VPM's B.N. Bandodkar College of Science, Thane, Maharashtra, India, in collaboration with the Department of Chemistry, The Institute of Science, Dr. Homi Bhabha State University Mumbai, India on 9th and 10th April, 2021.

Green chemistry aims to design and produce cost competitive chemical products and processes that attain the highest level of the pollution-prevention hierarchy by trying to reduce pollution at its source. Chemicals that are less hazardous to human health and the environment are less toxic to organisms. Green solvents can be used to improve chemical processes, mitigate the use of solvents and processing steps, and develop new routes and advancements that meets the requirements of sustainability due to its unique properties and functions.

This beginning will never stop till end, we are stimulating our goals and catalysing the research activities by taking help of chemical Gems (speakers) invited in our national conference ACSSD-2021. It will create novel thinking ability with respect to new openings, opportunities, guidance and direct relation between chemistry owners to chemistry world. This National conference platform would also provide a premier interdisciplinary forum to present and discuss the most recent innovations, trends, concerns and practical challenges encountered along with the solutions adopted in the form of invited talks, research paper presentations, poster presentations and discussions.

A platform like this will ignite a dialogue among all stakeholders and be useful in generating and inspiring young researchers. Organizing this National Conference was a great motivational experience for us, and it has been an incredible journey!!

-Dr. Sandeep Kahandal and Dr. Vikas Bangde

Organizing Secretary

Joint Organizing Secretaries' Address

We are delighted that Department of Chemistry, VPM'S Bandodkar College of Science, Thane and the Department of Chemistry, The Institute of Science, Dr. Homi Bhabha State University, Mumbai-32 are jointly organizing a "National Conference on Advances in Chemical Sciences and Sustainable Development (ACSSD-21) scheduled for during April 9-10, 2021.

The present conference is a unique opportunity to discuss and explore best practices within the teaching and laboratory research along with other related fields of chemistry. Further, it will open new doors of scientific works to face new challenges in 21st Century for the benefit of society. We trust that this event will provide a platform for researchers and participants to exchange their views and ideas. We extend our best wishes to the conference and all budding chemists and for the success of the event.

We wish the conference success.

-Dr. Ajit Bhumkar and Dr. Vishal Banewar

Joint Organizing Secretary

Students Representative Message

Respected Delegates,

It's our immense pleasure to welcome you all for virtual National Conference. The Conference topic is very much near to our thought of mind that is "ADVANCES IN CHEMICAL SCIENCE AND SUSTAINABLE DEVELOPMENT" (ACSSD 2021). This conference makes us to put forth, the main advantages of present study approach to eco-friendly nature in perspect of chemistry.

Often, it's difficult time, we students got such a golden opportunity to explore our maximum knowledge possible. It's been an absolute honour being student organizing member for the conference. And all the qualities that we have gained through this workshop and conferences will last forever in our mind

We would like to take this opportunity to thank our institute who has provided this platform for learning and believing in us and helping in all the possible ways. They don't only teach, they inspire. Also, would like to thanks all the eminent speakers for inspiring us, that really awakens our inner scientist.

Once again thanks to all!!!

Khan Hiba Masihul Haque
VPM's B.N Bandodkar college of Science,
(Autonomous) Thane (W)

Kanojiya Aparajita Chandrabhan
The Institute of Science,
Dr. Homi Bhabha State University Mumbai

FIRST PREPARATORY WORKSHOP OF NATIONAL CONFERENCE ON Advances in Chemical Sciences and Sustainable Development (ACSSD-2021)

Program Schedule

Saturday, February 6, 2021	Event
09.00 am to 09.05 am	Welcome address and about Department of Chemistry **Dr. D. R. Ambavadekar,** Head, Department of Chemistry VPMs B N Bandodkar College of Science, (Autonomous) Thane
09.05 am to 09.10 am	Welcome address and about Dr. Homi Bhabha State University **Dr. Gayatri Barbade,** Head, Department of Chemistry, Dr. Homi Baba State University The Institute of Science, Mumbai
09.10 am to 09.15 am	Opening Remark of Conference **Dr. A S. Goswami-Giri,** Associate professor and IQAC Coordinator VPMs B N Bandodkar College of Science, (Autonomous) Thane
09.15 am to 09.20 am	Conference Address by I/C Principal **Capt. (Dr). Moses Kolet** VPMs B N Bandodkar College of Science, (Autonomous) Thane
09.20 am to 09.25 am	Virtual Inauguration
Invited talk 1	
09.30 am to 10.20 am	**Prof. Shivram S. Garje** Professor, Associate Dean (Science and Technology) Department of Chemistry, University of Mumbai , Mumbai
Topic : Materials For Environmental Remediation and Sustainable Development	
Invited talk 2	
10:20 am to 11:10 am	**Anand Malankar** Research and Development Head, IFFCO – Personal Care Division. Dubai
Topic : Fragrance and Flavour Application Technology	
11.10 am to 11.50 am	Paper presentation by students
QA session by	
11.50 am to 12. 20 pm	**Dr.Rohini Mandhare** VPMs B N Bandodkar College of Science, Thane **Dr.Sushma Ambadekar,** Dr. Homi Baba State University The Institute of Science, Mumbai
12.20 pm to 12.25 pm	Vote of thanks **Dr. Sandeep Kahandal** VPMs B N Bandodkar College of Science, (Autonomous) Thane

SECOND PREPARATORY WORKSHOP OF NATIONAL CONFERENCE ON Advances in Chemical Sciences and Sustainable Development (ACSSD-2021)

Program Schedule

Saturday, March 6, 2021	Event
09.00 am to 09.02 am	Virtual Inauguration
09.03 am to 09.10 am	Welcome address and about Department of Chemistry **Dr. D. R. Ambavadekar** Head, Department of Chemistry VPMs B N Bandodkar College of Science, (Autonomous) Thane
09.10 am to 09.15 am	Welcome address and about Dr. Homi Bhabha State University **Prof. Yuvraj S. Malaghe** Joint Director, Mumbai Division and Head, Department of Chemistry, The Institute of Science , Mumbai, Dr. Homi Bhabha State University.
09.16 am to 09.20 am	Opening Remark of Conference **Dr. A S. Goswami-Giri** Associate professor and IQAC Coordinator VPMs B N Bandodkar College of Science, (Autonomous) Thane
09.21 am to 09.25 am	Conference Address by I/C Principal **Capt. (Dr). Moses Kolet** VPMs B N Bandodkar College of Science, (Autonomous) Thane
09.26 am to 09.35 am	Institutional Virtual Tour 1 and 2
Invited talk 1	
09.35 am to 10.25 am	**Dr. Hemantkumar S. Chandak** ASSOCIATE PROFESSOR in Chemistry and Coordinator- IQAC G. S. Science, Arts & Commerce College Khamgaon, Buldhana
Topic : Green synthesis of heterocyclic compounds using MCR and catalysis.	
10. 26 am to 10.40 am	QA -Interaction with speaker by **Mr. Nitin Gulvi** VPMs B N Bandodkar College of Science, Thane
Invited talk 2	
10:41 am to 11:30 am	**Prof. S. T. MHASKE** FMASc, HEAD, Department of Polymer & Surface Engineering Institute of Chemical Technology, Mumbai
Topic: Sustainability of Flexible Polymer Packaging.	
11:30 pm to 11.45 am	QA -Interaction with speaker By **Dr. Vikas M. Bangade** The Institute of Science, Mumbai, Dr. Homi Bhabha State University, Mumbai
11.46 am to 12.40 pm	Paper presentation by students
Vote of thanks	
12.41 pm to 12.50 pm	**Dr.Sushma Ambadekar,** Dr. Homi Bhabha State University, The Institute of Science, Mumbai

NATIONAL CONFERENCE ON Advances in Chemical Sciences and Sustainable Development (ACSSD-2021)

Program Schedule

Friday, 9th April 2021	Event (Day 1)
09.00 am to 09.02 am	Virtual Inauguration
09.02 am to 09.10 am	Institutional Virtual tour
09.10 am to 09.17 am	Welcome address by Convener of the Conference **Dr. D. R. Ambavadekar** Head, Department of Chemistry and Vice- Principal, VPM's B. N. Bandodkar College of Science, (Autonomous) Thane.
09.17 am to 09.24 am	Welcome address and about Dr. Homi Bhabha State University **Dr. Jairam M. Khobragade** Chair of the Conference and Director, The Institute of Science, Mumbai, Dr. Homi Bhaba State University, Mumbai.
09.24 am to 09.31 am	Conference Address by Convener in Chief **Capt. (Dr). Moses Kolet** I/C Principal, VPM's B. N. Bandodkar College of Science, (Autonomous) Thane.
09.31 am to 09.33 am	Inauguration of Proceedings of the Conference (ACSSD-2021)
09.33 am to 09.40 am	Patron Address **Dr. V. V. Bedekar** Chairman, Vidya Prasarak Mandal, Thane.
09.40 am to 09.47 am	Opening Remark of the Conference **Dr. A. S. Goswami-Giri** Co-Convener, Associate Professor and IQAC Coordinator VPM's B. N. Bandodkar College of Science, (Autonomous) Thane.
CHIEF GUEST	
09:47 am to 09:57 am	**Dr. Anthony Melvin Crasto** Worlddrugtracker, Principal scientist, Process research, Glenmark Pharmaceuticals Ltd, Navi Mumbai, India.
KEYNOTE ADDRESS	
09.57 am to 10.30 am	**Prof. Sanjio S. Zade** Professor, Chemical Sciences (DCS), IISER, Kolkata.
Topic: Thiophene containing ladder-type next-gen organic semiconductors.	
INVITED TALK – 1	
10:30 am to 11:20 am	**Prof. Vivek Polshettiwar** Associate Professor 'G', Department of Chemical Sciences, TIFR, Mumbai.
Topic: Nanochemistry for Sustainable Development.	
INVITED TALK – 2	

11.20 am to 12.10 pm	**Dr. Amit Zodge** R & D, Manager, Spice King Holland (SKH), Enschede, Netherlands
Topic: The Green Solvent-Supercritical CO_2 technology for Sustainable Chemistry.	
12.10 pm to 01.10 pm	Paper presentation (Oral/E-poster)
01.10 pm to 01.15 pm	Concluding Remarks **Dr. Gayatri Barbade** Head, Department of Chemistry, Dr. Homi Baba State University, The Institute of Science, Mumbai.
Saturday, 10th April 2021	**Event (Day 2)**
INVITED TALK – 3	
09:00 am to 09:50 am	**Dr. Muralidhar N. Ingale** Director, REYNISH PHARMACHEM PVT. LTD. Dabhasa, Vadodara, Gujarat, India.
Topic: Strategic approaches for optimizing performance and streamlining operations to foster quality and growth for Chemical Industry.	
INVITED TALK – 4	
09.50 am to 10.40 am	**Prof. Rajendra N. Shirsat** Department of Chemistry, Professor of Physical Chemistry, Goa University, Goa.
Topic: Topography of Molecular Electrostatic Potential.	
10.40 am to 12.00 pm	Paper presentation (Oral/E-poster)
12.00 pm to 12.30 pm	Valedictory function **Prof. A.D. Sawant** Former Vice Chancellor, University of Rajasthan, Jaipur Former Joint Director of Higher Education, Mumbai ; Former Pro Vice Chancellor, University of Mumbai
12.30 pm to 12.40 pm	**Glimpses of the conference**
12.40 pm to 12.50 pm	**Vote of Thank**

CONTENTS

Section III: Reports

SECTION I

KEYNOTE ADDRESS
&
INVITED TALKS

Keynote Address

Thiophene containing ladder-type next-gen organic semiconductors

Sanjio S. Zade
Department of Chemical Sciences, Indian Institute of Science Education and Research, Kolkata, Mohanpur 741246, Nadia, West Bengal, India.
Email: sanjiozade@iiserkol.ac.in

π-Conjugated systems that include conjugated small molecules and polymers have been an integral part of organic electronic devices such as organic photovoltaics (OPVs), organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and organic thermoelectrics (OTE). The general requirements for the use of organic semiconductors in printable, flexible electronic devices include (i) high chemical and thermal stability, (ii) high charge-carrier mobility, (iii) solution processability and (iv) easy synthetic routes. Apart from molecular design and synthesis, understanding molecular orbital engineering is an important aspect of creating the next-generation organic semiconductor. In this context, ladder/fused π-conjugated systems are fascinating candidates. In this talk, a synthetic approach to interesting ladder/fused conjugated systems and DFT approach to evaluate the properties of these systems will be discussed.

Invited talk

Materials for environmental remediation and sustainable development

Shivram S. Garje
Professor, Associate Dean (Science and Technology)
Department of Chemistry, University of Mumbai
Vidyanagari, Santacruz (East), Mumbai – 400098
Email: ssgarje@yahoo.com

With increasing industrialization and development of mankind, the threat to environment has increased. Also, the conventional energy sources are getting depleted. In view of this, there is need to prepare new materials which can be used for environmental remediation and sustainable development. This talk will cover synthesis of various nanomaterials and their applications in non-conventional energy sources, energy storage devices, degradation of organic pollutants, etc.

Invited talk

Fragrance and Flavour Application Technology

Anand Malankar
Research and Development Head, IFFCO - Persnal Care Division. Dubai
Email: anandmalankar74@gmail.com

DIVERSE ROLES IN PRODUCT POSITIONING AND MARKETING

Business Opportunity

- Farming Business – Growing of plants and herbs which yields natural Essential Oil and Perfumery compound
- Perfume oil Distillation
- Perfume Blending Factory
- Fine Fragrance / Body Spray & Deodorant Manufacturing Plant
- Trading
- Retails Sale
- **Career Opportunity**
- Perfumer
- Perfume Technologist
- Fragrance Development Manager
- Quality Controller
- Research & Development – New synthetic molecule

Fragrance’s main marketing roles are centered on three key themes: brand image, product targeting and the sensory experience. Under each of these headings, there are many more specific themes that fragrance can and does address.

Natural and organic personal care is still expanding its reach, particularly in developed markets, with even mainstream brands are being drawn to the natural theme. Extracts can also contribute to fragrance so there is a growing focus on more unusual and diverse botanical scents.

The Future of the Perfume Industry

- Today, perfumes are increasingly made using synthetic chemicals. Often, scents that occur naturally are reproduced synthetically rather than sourced and extracted. This allows the cost of producing perfume to go down
- Our sense of smell is the most powerful of the five senses, so it doesn’t look like perfumery is going away any time soon. The importance of scent has been around since the beginning of time, meaning smell is valuable for a multitude of purposes, including emotion, memory, creativity and relationships.
- Because of the significant impact of our olfactory sense on our daily lives, research is being conducted in the areas of synthetic human perfume (recreating human body scents i.e. pheromones) and aromatherapy. Perfume can go so far as to boost human emotional states and physical arousal.

- Today, perfumes are increasingly made using synthetic chemicals. Often, scents that occur naturally are reproduced synthetically rather than sourced and extracted. This allows the cost of producing perfume to go down
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Invited talk

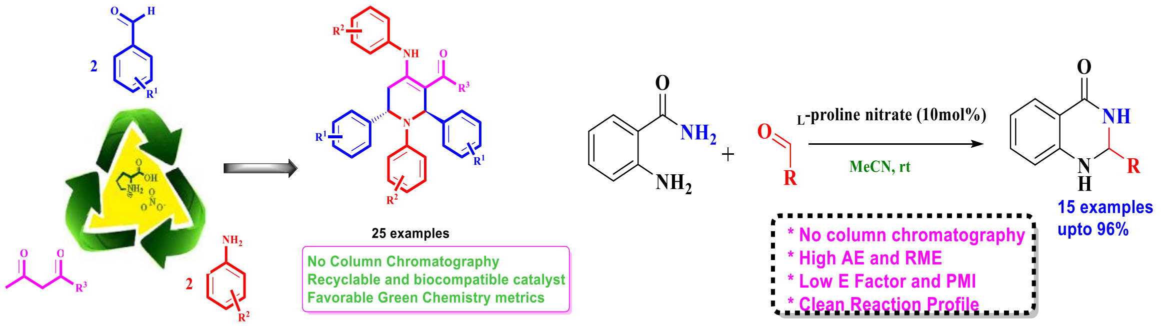
Green synthesis of heterocyclic compounds using MCR and catalysis

Hemantkumar S. Chandak
ASSOCIATE PROFESSOR in Chemistry and Coordinator- IQACG. S. Science, Arts & Commerce College Khamgaon, Buldhana

Email: chemants@gmail.com

Modern synthetic chemistry is usually measured by availability of simple, highly functionalized building blocks that can be used in the construction of complex molecules with diverse properties and applications. The synthesis of heterocycles using MCRs in a domain of classical carbonyl condensation chemistry has been an important synthetic strategy.

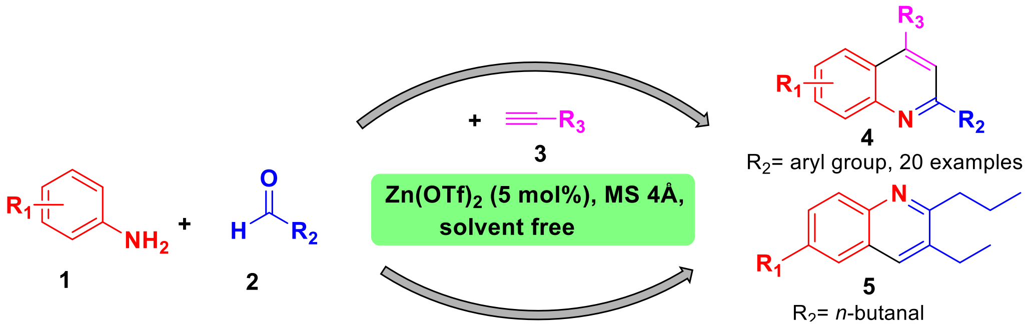
Homogeneous catalysis using ionic liquids (ILs) attracted great attention of the chemists in recent years. Commonly used ionic liquids, based on imidazolium cations and fluorinated anions are synthetic chemicals and have some inherent disadvantages. Our group explored the catalytic potential of L-proline nitrate as amino acid ionic liquid (AAIL) for the construction of various heterocycles. C-C, C-N and C-S bond formation can also be accomplished by employing L-proline nitrate. Synthesis of highly functionalized piperidines and 2,3-dihydroquinazolin-4(1*H*)-ones have been achieved using L-proline nitrate as AAIL (**Scheme 1**).



a) Highly functionalized piperidines b) 2,3-dihydroquinazolin-4(1*H*)-ones

Scheme 1: L-proline nitrate in the construction of C-C and C-N bond formation

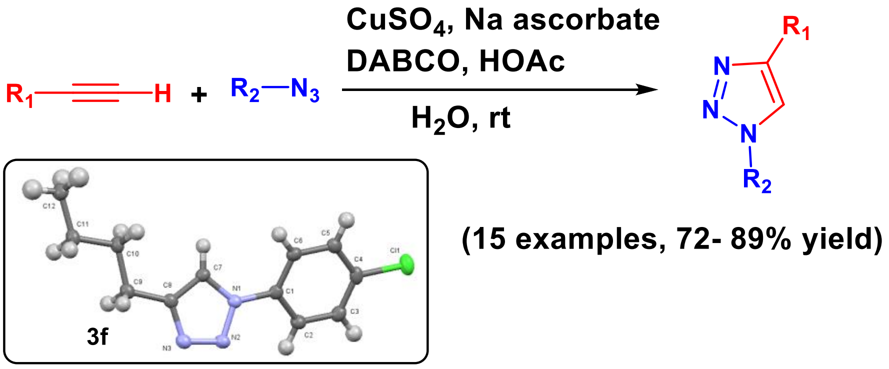
Heterogeneous catalysis using Zn(OTf)$_2$ for the multi-component, solvent-free synthesis of quinolines via C-H activation of alkynes also being explored by our group (**Scheme 2**).



Scheme 2: Zn(OTf)$_2$-mediated synthesis of aryl/alkyl substituted quinolines

Carbon- heteroatom bonds are much more frequently occurring in nature than carbon-carbon bonds, which is plausible considering that carbon dioxide is nature's main building block and water the reaction medium. The most important structural units, nucleic acids, proteins and polysaccharides are all condensates of monomers that are linked *via* carbon-heteroatom bonds. However, nature had almost infinite resources of time and materials to create this fascinating universe of enzymatically controlled interdependent reaction pathways. For chemists, who have very limited resources and no home-tailored enzymes to control their reactions, carbonyl chemistry is a very demanding field. On the one hand, there is hardly any thermodynamic driving force in carbonyl chemistry. In particular, equilibrium 'aldol' reactions are often energetically favorable by less than 3 kcalmol^{-1}. For the completion of such processes, an additional 'push' must be provided, often by application of Le Chatelier's principle (for example, azeotropic removal of water), by coupling the desired process to an exothermic co-reaction (for example, a strong 'base' or a strong 'acid'), or by virtue of favorable entropic considerations (such as intramolecular ring closure) without enthalpic penalties (such as formation of strained rings). Only with the advent of kinetically controlled enolate chemistry has aldol chemistry become a powerful and selective synthetic tool. However, the use of strong bases such as lithium diisopropylamide (LDA) necessitates the application of protecting groups for other functional groups. This development turned total synthesis into a complicated business. Based on these observations, Sharpless and co-workers propose a renunciation from this path of applying complicated and long organic syntheses for the preparation of most challenging carbon frameworks, and ask for a return to the basic task of creating new substances with the desired profile of properties and functions. This is the philosophy that triggered the development of "Click" chemistry.

Copper catalyzed azide-alkyne cycloaddition (CuAAC) has been a cream crop of click chemistry since Huisgen [3+2] cycloaddition under catalytic condition was rediscovered independently by the groups of Sharpless and Meldal. Electron deficient azides are challenging substrates since they do not very frequently provide the corresponding 1,2,3-triazoles. N-sulfonyl azides usually reacts with alkyne in presence of corresponding catalytic system giving amidines, imidates, or amides via the reaction of ketinimine intermediate with variety of nucleophiles. With an aim to design a simple, efficient and expeditious protocol that should be modular with respect aryl-/ alkyl-/ sulfonyl- azides, we employed 1,4-diazabicyclo(2.2.2) octane (DABCO) and acetic acid accelerated aqueous ascorbate method for synthesis of 1,4-substituted 1,2,3-triazole (**Scheme 3**).



Scheme 3: DABCO-HOAc jointly Accelerated CuAAC on water

Invited talk

Sustainability of Flexible Polymer Packaging

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To be genuinely described as sustainable a product or material, it must be environmentally, economically and socially sustainable. The three pillars of sustainability have become known as the three. All three pillars of sustainability have a positive impact on plastics. The environmental profile in plastics is very good. Only 4% of world production of oil for plastics is used, and much less energy than other materials is used to produce it. Plastics are durable and lightweight, thus reducing weight in cars, planes, packaging and piping. As a packaging material, plastics offer unparalleled advantages. This is due to the lightweight, efficient resource and excellent obstacle characteristics of plastics. These characteristics reduce waste and save energy considerably in packaging items in plastics.

Invited talk

Nanochemistry for Sustainable Development

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“Life -the most complex form of matter in the universe – is on course for its inevitable extinction, unless we humans, the chosen ones, can agree to live within the limits of nature’s rules”. Disproportionate use (or misuse) of natural resources, including fossil fuels, created an extreme imbalance on planet earth and the first priority of all of us to take on this challenge.

Running your car for a lifetime by just filling CO_2 only once could be possible if we can capture and convert CO_2 to methane. In this talk, I will discuss some of our work in the Field of Catalysis & Nanochemistry, such as DFNS, Black Gold, Defective Nanosilica and Solid Acids to combat climate change.

Invited talk

The Green Solvent-Supercritical CO_2 technology for Sustainable Chemistry

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Abstract:

Effective enatiomeric separation and purity of individual form using environmentally benign solvent is a topic of great interest for pharmaceuticals and food industry due to the different biological activity. Hence we studied the diastereomeric salt formation of racemic 2-methoxyphenylacetic acid (MPAA) with enantiopure (R)-(-)-1- cyclohexylethylamine (CHEA) using gas antisolvent approach in supercritical carbon dioxide (CO_2). 45% enatiomeric enrichment along with 60% yield was achieved at 120 bar CO_2 and 40°C for 1 hour reaction time.

Successfully synthesized the highly crystalline new enantiopure salt of S-MPAA and S-CHEA using supercritical CO_2. Parametric studies such as effect of different molar ratios, solvents, pressures and temperatures on diastereomeric salt formation reaction were also studied in detailed. Higher crystanality is observed on use of supercritical CO_2.

Reaction procedure involved the dissolution of specific molar ratio of racemates and resolving agent in minimum amount of solvent to form homogeneous phase. These homogeneous phases further allow to react in high pressure autoclave pressurize with supercritical CO_2. Constant temperature is maintained by using the jacketed thermo bath.

After the reaction, extraction was done with 3-fold volume of supercritical CO_2 with respect to reactor volume. Formed reaction products i.e. raffinate and extract were analyzed for quantification. Diastereomeric salt precipitated as a raffinate in the reactor vessel. Main constituents of extract are unreacted starting materials and used organic solvents. Several polar, non-polar and its mix composition solvents were screen. Polarity was tuned on mixing of polar and non-polar solvent in certain proportions. Among all combinations Acetonitrile and Toluene (1:1) mixture, found to be effective.

From 1:1, 2:1 and 1:0.25 molar ratio study it is revealed that the half equivalent method (2:1) or commonly known as the Pope-Peachy method is suitable for the resolution of racemic MPAA using (R)-(-)-CHEA. No remarkable change in enantiomeric excess or yield was observed with further increase in temperature and pressure. Formed diastereomeric salt were characterized using capillary electrophoresis (CE), differential scanning calorimetry (DSC), Fourier transform infrared spectroscopy (FTIR) and X-ray powder diffraction (XRD).

XRD study confirms the formation of new crystalline diastereomeric salt species. DSC study of diastereomeric salt showed reasonably higher and new melting pattern. FTIR Study supports the formation of acid-amine diastereomeric salt.

Acknowledgements:

This research work was supported by DoHip Network, European Community's Seventh Framework Programme (FP7) under grant agreement no: 316959.

Keywords: Diastereomeric salt, Gas antisolvent, Supercritical CO2, Enantiopure compound, chiral resolution

References:

1) Kenichi Sakai, Masami Yokoyama, Rumiko Sakuraia and Noriaki Hirayama, *Tetrahedron: Asymmetry* 17 1541–1543 (2006).

2)Takuji Hirose, Muksana Begum, M. Sdequl Islam, Kayoko Taniguchi, Mikio Yasutake, *Tetrahedron: Asymmetry* 19 1641–1646 (2008).

3) Rumiko Sakurai, Atsushi Yuzawa , Kenichi Sakai, *Tetrahedron: Asymmetry* 19 1622 1625(2008).

4) György Bánsághi, Edit Székely, David Méndez Sevillano, Zoltán Juvancz, Béla Simándi, *J. of Supercritical Fluids* 69 113– 116 (2012).

Invited talk

Strategic approaches for optimizing performance and streamlining operations to foster quality and growth for Chemical Industry

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Sustainabilities strategies in today's chemical industry have the aim to minimize negative social and environmental impacts associated with chemical production by developing innovative and eco-friendly products and services while continuing to meet customer and consumer needs. To achieve this goal, careful environmental impacts including emission of air and GHGs, intensity of energy and water use must be handled. Companies have found that sustainability initiatives can make significant savings through the reduction of energy, water and feedstocks overheads. Many chemical companies have already acknowledged the reduction of emissions as an opportunity to gain more efficiency and reduce costs, potentially distracting the sector from the forecast of growth.

Invited talk

Topography of Molecular Electrostatic Potential

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Molecular Electrostatic Potential (MESP) is a interaction energy of a unit positive charge with a molecule. This energy takes a positive value near the nuclear framework and negative value at electron rich sites being a continuous function it also attains zero values. This property can be used to locate electron rich sites for molecules (like lone pairs of electrons, double bonds etc.) to see the sites of electrophilic attacks. Sites of nucliophilic attacks can also be seen by obtaining this property on a predefined surface (iso-density surface). Visualization of this three dimensional property plays a vital role in qualitative analysis of molecular property. Quantitative analysis may be obtained by making use of topographical study of this three dimensional function. Numerous articles on the use of MESP in inorganic, organic and medicinal chemistry have appeared in popular scientific journals. Reviews, Books and monographs have also been published recently on the applications of Molecular Electrostatic Potential.

The goal here is to make use of various topographical features of electrostatic potential of molecules such as minima and saddle points to understand intermolecular interaction which is one of major area of quantitative structure activity relationship (QSAR) in computational chemistry.

Keywords:

Electrostatic potential, Topography of scalar fields, Visualization of functions, QSAR.

Reference:

Electrostatics of atoms and molecules, Shridhar R Gadre, Rajendra N Shirsat, Universities Press, 2000

SECTION II

RESEARCH PAPERS

Synthesis and Antimicrobial Activity of Novel Benzofuran Derivatives

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Abstract

Dehydrodiisoeugenol constitute a new group of antimitotic and potential anticancer agents that inhibit tubulin polymerization. It is a benzofuranoid type neolignan have been synthesized by oxidative coupling of isoeugenol and diversified to its respective ether (K_2CO_3 / Acetone / Alkyl / Aryl halide) derivatives using conventional methods and characterized by ^1H NMR, elemental analysis and mass spectral data. These synthesized compounds were screened for their potential antibacterial activity against Gram-positive and Gram-negative cultures. Few of them possess promising antibacterial activity.

Keywords

Dehydrodiisoeugenol, ^1H NMR, TOF MS, Gram-positive and Gram-negative cultures, antibacterial.

Introduction

Heterocyclic synthesis has emerged as powerful technique for generating new molecules useful for drug discovery[1]. Heterocyclic compounds provide scaffolds on which pharmacophores can arrange to yield potent and selective drugs[2]. Eg. Cabazitaxel, Eribulin. Benzofuran are the important group of heterocyclic compounds, several derivatives of which have been marked as biologically and pharmacologically active product. The literature survey revealed that, benzofuran also possess different biological activities such as antibacterial[3], antifungal[4], anti-inflammatory[5], antidepressant[6], analgesic[7] and hypoglycemic activities[8]. Eg. Amiodarone, Angelicin, Bergapten. In the present work, we are synthesizing dehydrodiisoeugenol[9] by subjecting isoeugenol to oxidative coupling using iodobenzene diacetate in dichloromethane. It also shows pronounced antileishmanial, antiplasmodial activities and served as a suitable starting material for the synthesis of various bioactive molecules such as fragnasol B. Since it possesses various biological activities and in continuation to our earlier work[10-12] we decided to make a library of compounds using various permutation and combinations to come up with novel ether derivatives of dehydrodiisoeugenol using conventional methods for better activities. The objective of this study is to condense two molecules of the same disease domain to produce more potent candidate in the same disease domain or to condense two molecules of different disease domain to produce mixed variety of those disease domain or to have drug candidate with entirely different biological activity.

Materials and methods

Materials: Chemicals used were of a laboratory grade. The reactions were monitored by TLC on aluminium-backed silica plate visualized by UV-light.

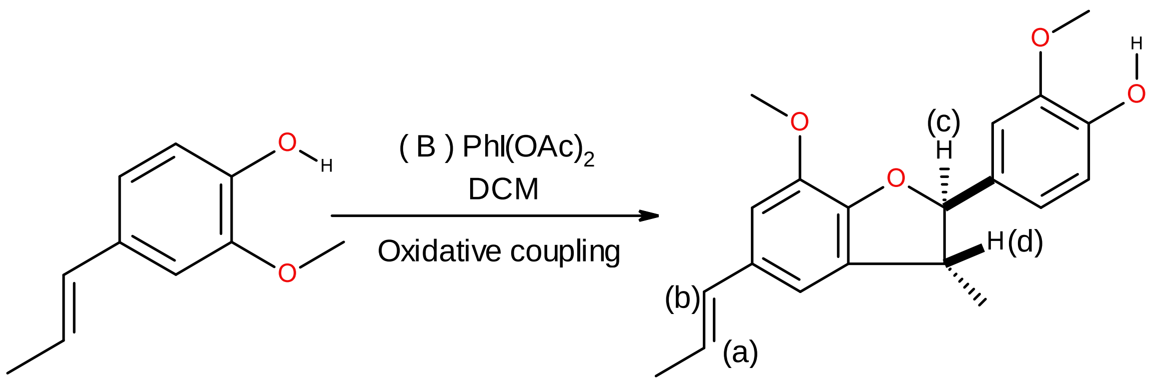
Experimental

Melting points were determined on a Thomas Hoover capillary melting point apparatus using digital thermometer. IR spectra were recorded on a Shimadzu FTIR Prestige model as KBr pellet. ^{1}H NMR spectra were recorded on a Varian 400 MHz spectrometer in $CDCl_3$. Chemical shifts were recorded in parts per million down field from tetramethyl silane. Mass spectra were recorded on a TOF MS ES mass spectrometer. Elemental analysis was carried out as a percentage on a Thermo finnigan, Flash EA 1112 series, Italy.

Results and discussion

Synthesis of Dehydrodiisoeugenol:- To a stirred solution of [A] (4.0 g, 24.35 mmol) in dichloromethane (75 ml) was added dropwise a solution of IDA (2.5 g, 7.76 mmol) in dichloromethane (100 ml) at room temperature within 4 h and stirring was continued at room temperature for 48 h. Subsequently the same amount of IDA in dichloromethane (100 ml) was added within 4 h. After stirring, the reaction mixture at room temperature for 2 h., 3 g of solid $NaHCO_3$ was added and the stirring was continued for 5 h. Subsequently, $NaHCO_3$ was filtered off, and the solvent was evaporated to give a yellow oil, whose purification by flash chromatography on silica gel (n-hexane : ethyl acetate, 6 : 1) resulted in [C](1.4 g, 38 %) as white needles with m.p. 132 – 133^{0}C. ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 from isoeugenol moiety), 3.4 – 3.5 (m, 1H, proton 'd'), 3.87 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 5.10 (d, J = 9.2 Hz, 1H, -benzylic proton 'c'), 5.64 (s, 1H, -OH, D_2O exchangeable), 6.0 – 6.2 (m, 1H, olefinic proton 'a'), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton 'b'), 6.7 – 7.1 (m, 5H, ArH).

Reaction scheme 1 :

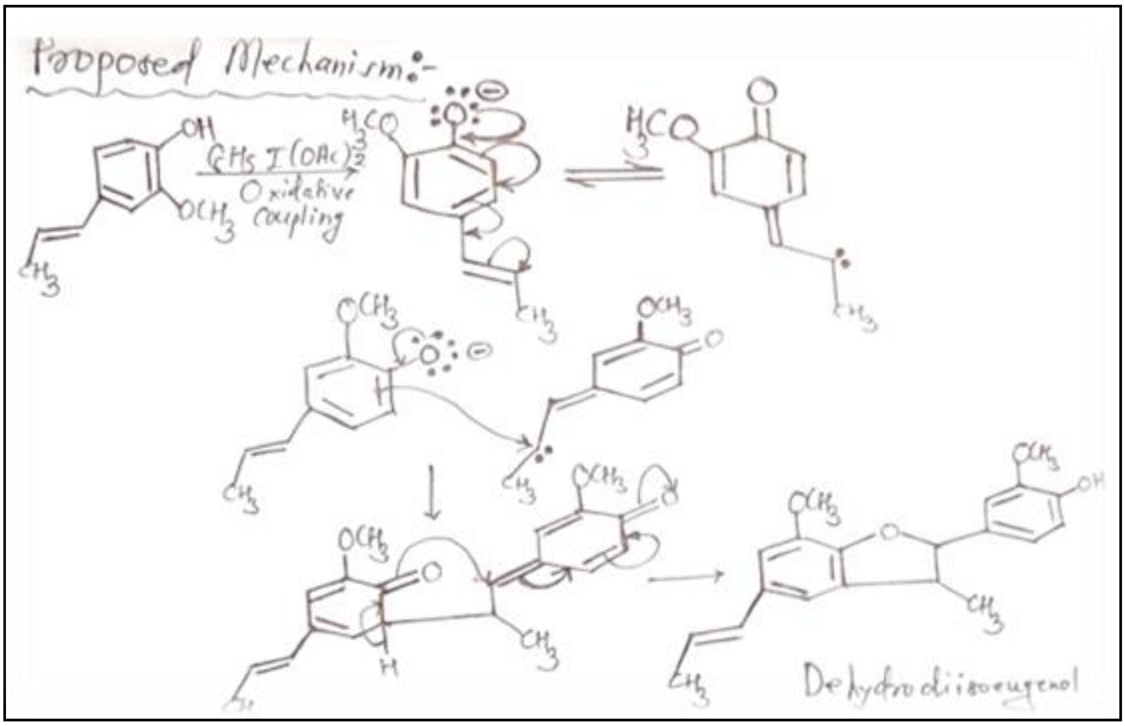


(A)

Isoeugenol

(C)

Dehydrodiisoeugenol



Diversification of Dehydrodiisoeugenol {2-methoxy-4-[7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydro-1-benzofuran-2-yl]phenol} to its ether derivatives:- Compounds (1) to (9) [Table 1] were synthesized by following general method.

To a stirred solution of [A] (1 eq.) In 30 ml acetone was added [B] (2.5 eq.) And stirring continued at 40^0C for next 30 min. For complete formation of K-salt. To this compound [C] (2 eq.) Was added and stirring continued at 45 – 50^0C for next 8 h. The progress of the reaction is monitored by TLC for the completion of the reaction.

Work up: - The reaction mixture filtered through Buchner funnel, wash the cake with 25 ml acetone. The total organic layer was concentrated to minimum, preabsorbed on silica gel and purified by silica gel (100 – 200 mesh) column chromatography with increase in concentration of ethyl acetate in petroleum ether. The general yields range between 60 – 80 %.

The most significant features of this methodology are (a) good accessibility of the reagent and its stability (b) a stoichiometric amount of reagent can be used by direct weighing, avoiding excess (c) no evolution of hazardous vapours during the reaction (d) the total elimination of the use of toxic organic solvents (e) a simple experimental procedure (g) good control over the outcome of the reaction by varying the amount of reagent (h) less expensive and (i) very simple reaction work up with avoidance of by-product. The aforesaid protocol thus provides an improved procedure for the synthesis of useful hybrid derivatives having important pharmaceutical, agricultural and other physicochemical properties.

Reaction scheme 2 :

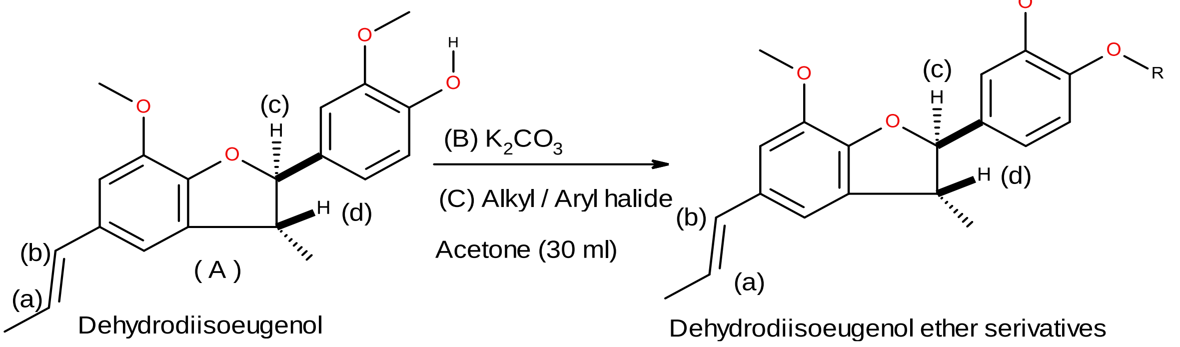
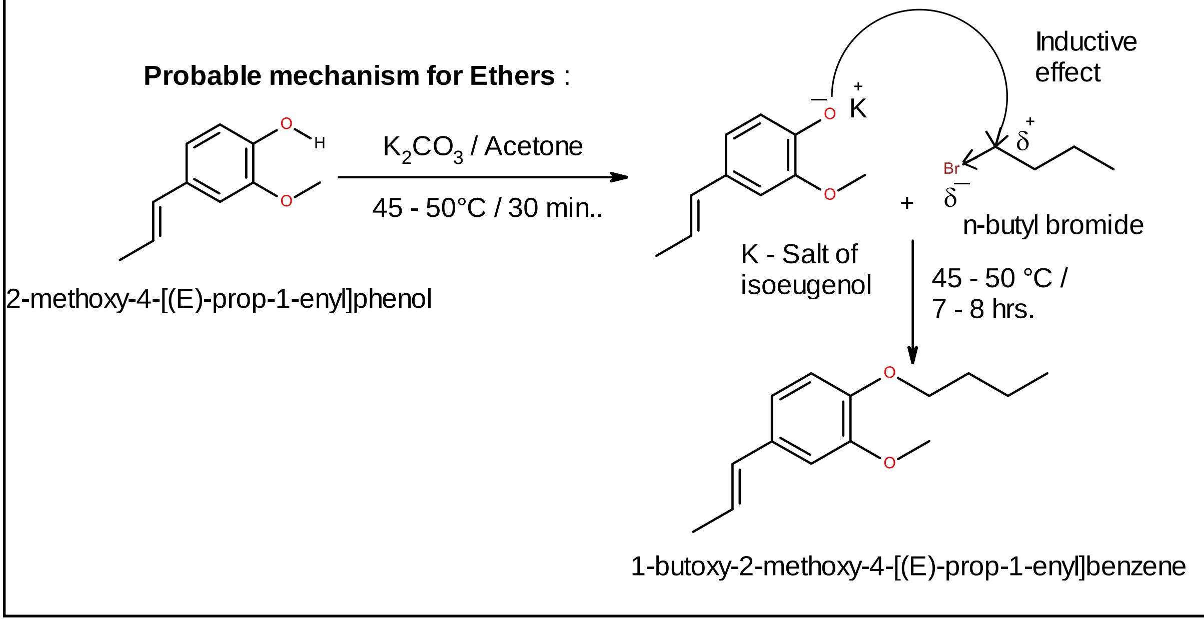


Table 1: Dehydrodiisoeugenol ether derivatives.

Compound No.	R
1	Methyl
2	Ethyl
3	Propyl
4	Allyl
5	Butyl
6	Heptyl
7	Dodecyl
8	Acetone
9	Benzyl

Taking Isoeugenol as general example, the probable mechanism for ethers can be given as follows.

Probable mechanism for Ethers :



Chromatographic system

Column chromatography: For column chromatography 100 – 200 mesh Acme grade silica gel is used. The crude reaction mixture is concentrated under reduced pressure to yield crude mass which is preabsorbed on silica gel and purified by column chromatography with increase in concentration of Ethyl acetate in Petroleum ether. The fractions having similar ‘R_f” values were pooled together, concentrated and subjected for characterization using various spectroscopic techniques.

Thin layer chromatography: TLC plates were prepared using silica gel G (ACME, BOMBAY). Pet. Ether: etoac (85: 15) was used as the solvent system.

Radial chromatography: The circular glass plates of thickness 1 mm, were prepared by using silica gel (PF254, E. MERCK, 50 g) in cold distilled water (105 ml). For elution, gradually increasing concentrations of etoac in pet ether were employed.

Characterization of compounds (1 - 9): -

(1) (2R,3R)-2-(3,4-dimethoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran:-

Off white solid; Molecular Formula $C_{21}H_{24}O_4$; Melting Range 118 – 120^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$)∂_{ppm} :- 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 from isoeugenol moiety), 3.4 – 3.5 (m, 1H, proton ‘d’), 3.87 (s, 3H, Ar x –OCH_3), 3.88 (s, 3H, Ar x –OCH_3), 3.90 (s, 3H, Ar x –OCH_3), 5.11 (d, J = 9.2 Hz, 1H, -benzylic proton ‘c’), 6.0 – 6.2 (m, 1H, olefinic proton ‘a’), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton ‘b’), 6.7 – 7.0 (m, 5H, ArH); TOFMS : 341 (M + H); Elemental Analysis, Requires C 74.09 % H 7.11 % O 18.80 % Found C 74.11 % H 7.07 % O 18.77 %.

(2) (2R,3R)-2-(4-ethoxy-3-methoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran:-

Off white solid: Molecular Formula $C_{22}H_{26}O_4$; Melting Range 119 – 121^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 1.38 (d, J = 6.8 Hz, 3H, -$\mathbf{CH_3}$), 1.45 (t, J = 7.0 Hz, 3H, -O$\mathbf{CH_2}CH_3$), 1.86 (d, J = 6.7 Hz, 3H, -terminal –CH_3 frpm isoeugenol moiety), 3.4 – 3.5 (m, 1H, proton ‘d’), 3.86 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 3.90 (s, 3H, Ar x –OCH_3), 5.10 (d, J = 9.2 Hz, 1H, -benzylic proton ‘c’), 6.0 – 6.2 (m, 1H, olefinic proton ‘a’), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton ‘b’), 6.7 – 7.0 (m, 5H, ArH); TOFMS : 355 (M + H); Elemental Analysis, Requires C74.55 % H 7.39 % O 18.06 % Found C 74.52 % H 7.36 % O 18.10 %.

(3) (2R,3R)-2-(4-propoxy-3-methoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran:-

Off white solid: Molecular Formula $C_{23}H_{28}O_4$; Melting Range 78 – 80^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 1.03 (t, J = 7.4 Hz, 3H , -$\mathbf{CH_3}$ from n-propyl moiety), 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 frpm isoeugenol moiety), 1.8 – 2.0 (m, 2H, -$OCH_2\mathbf{CH_2}CH_3$ from n-propyl moiety), 3.4 – 3.5 (m, 1H, proton ‘d’), 3.86 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 3.97 (t, J = 7.0 Hz, 2H, -**OCH_2**CH_2CH_3 from n-propyl moiety), 5.11 (d, J = 9.2 Hz, 1H, -benzylic proton ‘c’), 6.0 – 6.2 (m, 1H, olefinic proton ‘a’), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton ‘b’), 6.7 – 7.0 (m, 5H, ArH); TOFMS : 369 (M + H); Elemental Analysis, Requires C74.96 % H 7.66 % O 17.37 % Found C 74.92 % H 7.63 % O 17.40 %.

(4) (2R,3R)-2-(4-allyloxy-3-methoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran: -

Off white solid; Molecular Formula $C_{23}H_{26}O_4$; Melting Range 108 – 110^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 frpm isoeugenol moiety), 3.4 – 3.5 (m, 1H, proton ‘d’), 3.86 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 4.61 (d, J = 6.0 Hz, 2H, -O**CH_2**-), 5.10 (d, J = 9.2 Hz, 1H, -benzylic proton ‘c’), 5.27 (m, 1H, olefinic proton from allyl moiety), 6.0 – 6.2 (m, 1H, olefinic proton ‘a’), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton ‘b’), 6.7 – 7.0 (m, 5H, ArH); TOFMS : 367 (M + H); Elemental Analysis, Requires C75.38 % H 7.15 % O 17.46 % Found C 75.35 % H 7.12 % O 17.50 %.

(5) (2R,3R)-2-(4-butoxy-3-methoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran: -

Off white solid; Molecular Formula $C_{24}H_{30}O_4$; Melting Range 75 – 77^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 0.97 (t, J = 7.4 Hz, 3H , -**CH_3** from n-butyl moiety), 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.4 – 1.6 (m, 2H, -**CH_2** from n-butyl moiety), 1.75 – 1.85 (m, 2H, -**CH_2** from n-butyl moiety), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 from isoeugenol moiety), 3.4 – 3.5 (m, 1H, proton ‘d’), 3.85 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 4.02 (t, J = 6.3 Hz, 2H, -**OCH_2** from n-butyl moiety), 5.12 (d, J = 9.2 Hz, 1H, -benzylic proton ‘c’), 6.0 – 6.2 (m, 1H, olefinic proton ‘a’), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton ‘b’), 6.7 – 7.0 (m, 5H, ArH); TOFMS : 383 (M + H); Elemental Analysis, Requires C75.36 % H 7.81 % O 16.73 % Found C 75.32 % H 7.77 % O 16.77 %.

(6) (2R,3R)-2-(4-heptoxy-3-methoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran: -

Off white solid; Molecular Formula $C_{27}H_{36}O_4$; Melting Range 85 – 87^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 0.89 (t, J = 7.0 Hz, 3H , -**CH_3** from n-heptyl moiety), 1.2 – 1.6 (m, 8H, 4 x –CH_2 from n-heptyl moiety), 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.75 – 1.85 (m, 2H, -**CH_2** from n-heptyl moiety), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 from isoeugenol moiety), 3.4 – 3.6 (m, 1H, proton ‘d’), 3.85 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 4.0 (t, J = 6.3 Hz, 2H, -**OCH_2** from n-heptyl moiety), 5.11 (d, J = 9.2 Hz, 1H, -benzylic proton ‘c’), 6.0 – 6.2 (m, 1H, olefinic proton ‘a’), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton ‘b’), 6.7 – 7.0 (m, 5H, ArH); TOFMS : 425 (M + H); Elemental Analysis, Requires C76.38 % H 8.55 % O 15.07 % Found C 76.35 % H 8.52 % O 15.10 %.

(7) (2R,3R)-2-(4-dodecoxy-3-methoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran: -

Off white solid: Molecular Formula $C_{32}H_{46}O_{4}$; Melting Range 127 – 129^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 0.88 (t, J = 7.3 Hz, 3H , -**CH_3** from n-dodecyl moiety), 1.2 – 1.6 (m, 16H, 8 x –CH_2 from n-dodecyl moiety), 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.75 – 1.85 (m, 2H, -**CH_2** from n-dodecyl moiety), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 from isoeugenol moiety), 3.41 (t, J = 7.3 Hz, 2H, -**CH_2** from n-dodecyl moiety), 3.3 – 3.5 (m, 1H, proton 'd'), 3.85 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 4.0 (t, J = 7.3 Hz, 2H, -**OCH_2** from n-dodecyl moiety), 5.10 (d, J = 9.7 Hz, 1H, -benzylic proton 'c'), 6.0 – 6.2 (m, 1H, olefinic proton 'a'), 6.36 (d, J = 15.9 Hz, 1H, -olefinic proton 'b'), 6.7 – 7.0 (m, 5H, ArH). TOF-MS: 495 (M + H); Elemental Analysis, Requires C77.69 % H 9.37 % O 12.94 % Found C 77.66 % H 9.33 % O 12.98 %.

(8)1-[2-methoxy-4-[(2R,3R)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran -2-yl]phenoxy]propane-2-one:-

Off white solid; Molecular Formula $C_{23}H_{26}O_{5}$; Melting Range 98 – 100^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 1.38 (d, J = 6.8 Hz, 3H, -CH_3), 1.86 (d, J = 6.6 Hz, 3H, -terminal –CH_3 frpm isoeugenol moiety), 2.28 (s, 3H, -CO**CH_3** from monochloro acetone moiety), 3.4 – 3.5 (m, 1H, proton 'd'), 3.87 (s, 3H, Ar x –OCH_3), 3.89 (s, 3H, Ar x –OCH_3), 4.58 (s, 2H, -**OCH_2** from monochloro acetone moiety), 5.10 (d, J = 9.2 Hz, 1H, -benzylic proton 'c'), 6.0 – 6.2 (m, 1H, olefinic proton 'a'), 6.35 (d, J = 15.7 Hz, 1H, -olefinic proton 'b'), 6.7 – 7.1 (m, 5H, ArH). TOF-MS: 383 (M + H); Elemental Analysis, Requires C72.23 % H 6.85 % O 20.92 % Found C 72.20 % H 6.82 % O 20.96 %.

(9) (2R,3R)-2-(4-benzyloxy-3-methoxy phenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran: -

Off white solid: Molecular Formula $C_{27}H_{28}O_{4}$; Melting Range 118 – 120^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$) ∂_{ppm} :- 1.37 (d, J = 6.7 Hz, 3H, -**CH_3**), 1.86 (d, J = 6.5 Hz, 3H, -terminal –CH_3 from isoeugenol moiety), 3.4 – 3.5 (m, 1H, proton 'd'), 3.87 (s, 3H, Ar x –OCH_3), 3.88 (s, 3H, Ar x –OCH_3), 5.10 (d, J = 9.2 Hz, 1H, -benzylic proton 'c'), 5.15 (s, 2H, -O**CH_2**Ph i.e. benzylic –O**CH_2**), 6.0 – 6.2 (m, 1H, olefinic proton 'a'), 6.36 (d, J = 15.8 Hz, 1H, -olefinic proton 'b'), 6.7 – 7.0 (m, 5H, ArH), 7.2 – 7.5 (m, 5H, ArH from benzyl bromide moiety); TOFMS : 416 (M + H); Elemental Analysis, Requires C 77.86 % H 6.78 % O 15.37 % Found C 77.82 % H 6.80 % O 15.40 %.

Biological activity

Antibacterial Activity using ditch plate method[13]:- The synthesized molecules were screened for their antibacterial activity using ditch plate method at 100 µg / ml concentration against Gram positive (*Staphylococcus aureus, Corynebacterium diphtheriae*) and Gram negative (*Escherichia coli, Salmonella typhi, Proteus vulgaris*) bacterial species qualitatively.

Theory: Ditch plate method is the method of chosen to test the anti-bacterial activity of compounds. It is a preliminary method to screen the anti-microbial potential of compounds /drugs, which are insoluble or partially soluble in aqueous phase. In this method, the test compound is seeded in an agar plate and the test organisms are streaked across to test the inhibition of the growth as a marker of anti-microbial activity.

Procedure: A ditch (10 mm x 70 mm) is cut into sterile MH agar plate. The test drug /compound is added to 5 ml molten MH agar butt at 400C and this mixture is poured into the ditch and allowed to solidify. The ditch should be made in level with the rest of the agar by pouring the mixture. The different bacterial cultures are streaked perpendicular to the ditch using nichrome wire loop. The plate is then incubated at 37^0 C for 24 hours. The results are observed as inhibition of bacterial growth on the ditch as well as adjacent to the ditch. The following test samples showed antibacterial activity against the organisms mentioned in the following **Table 2**.

Table 2: Antibacterial Activity Results

Sample No.	Active Against
Dehydrodiisoeugenol	*Staphylococcus aureus* [Gram positive] *Salmonella typhi* [Gram negative] *Klebsiella pneumoniae* [Gram negative] *Corynebacterium diphtheriae* [Gram positive] *Escherichia coli* [Gram negative]
1	*Staphylococcus aureus* [Gram Positive] *Escherichia coli* [Gram negative]
3	*Staphylococcus aureus* [Gram Positive] *Proteus vulgaris* [Gram negative] *Salmonella typhi* [Gram negative]
7	*Staphylococcus aureus* [Gram positive] *Salmonella typhi* [Gram negative] *Klebsiella pneumoniae* [Gram negative] *Corynebacterium diphtheriae* [Gram positive] *Escherichia coli* [Gram negative]
9	*Staphylococcus aureus* [Gram positive] *Escherichia coli* [Gram negative]

The novel hybrid derivatives of dehydrodiisoeugenol were synthesized by cost effective industry viable process following the principle of green chemistry in a reasonably good yield. The probable mechanism for the formation of ether derivative was also discussed.

The biological activity suggests that the base molecule dehydrodiisoeugenol have anti-bacterial activity against both the bacterial cultures. Its derivatives *viz.* 1, 3, 7 and 9 were also active against certain Gram + ve and Gram – ve cultures. Thus, ether derivatives of dehydrodiisoeugenol (1, 3, 7, 9) were potential antibacterial candidates. In depth analysis of these compounds through structure activity relationship studies would provide further insight and can be an interesting topic of future studies.

Conclusion

The structural diversity and the pronounced biological activities encountered in the benzofuran derivatives suggests that this class of compounds is worthy for further studies that may lead to derivatives by using combinatorial chemistry approach is an alternative strategy to new therapeutic discovery. In other words, the generation of diverse benzofuran derivatives develop new therapeutic molecules that might result in candidates having better activity.

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Lipid Peroxidation Studies and Antioxidant Activity of Glutathione Reductase in Crucian Carp Exposed to Heavy Metal Toxicity

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Abstract

The quality of the environment is waning because of the accumulation of several pollutants either in directly or indirectly. Heavy metal pollution is one among the harmful pollutions, which deteriorate the soft tissues and undergo bioaccumulations even in hard tissues like bones. Through food chain the heavy metals ultimately reach the humans and cause similar effects within the lower animals. Along with several other studies biochemical aspects of antioxidants under the physiological stress as induced by heavy metals is well reported in fish. It is demonstrated that the heavy metals can increase oxidative stress which may result into lipid peroxidation. In the present investigation, an effort was made to assess the effect of lead and mercury on oxidative stress and antioxidant enzymes in the liver tissue of Crucian carp (Carassius auratus). The fish were exposed to sub lethal dose of 96 hr LC50 of lead and mercury for 7 days and 21 days. A recovery set was separately maintained. The tissue was examined for lipid peroxidation (LPO) and Reduced glutathione (GSH). The present study of metal treated fish shows the increased level of lipid peroxidation and decreased level of reduced glutathione (GSH) within the liver tissue of fish goldfish.

Keywords

Crucian carp, oxidative stress, LPO, GSH, Heavy metals.

Introduction

Fish, in comparison with other aquatic invertebrates are more susceptible and heavily exposed to heavy metals toxicity as they live and feed in water (Saleh, 2014). They are more sensitive to many toxicants and are a convenient test subject for indication of ecosystem health. Heavy metals are produced from a variety of natural and anthropogenic sources (Garcia,2015). Out of the various types of anthropogenic activities, coal combustion is one of the most important process for the emission of trace elements and an important source of a number of metals (Wagner A.,2003). The contamination of heavy metals and metalloids in water and sediment, when occurring in higher concentrations, is a serious threat because of their toxicity, long persistence, and bioaccumulation and bio magnification in the food chain (Eisler R,1993). Fish are considered to be the most significant bioindicators in estimating the increased levels of heavy metals and understanding the changes in the environment by the physiological stress that they undergo due to heavy metal toxicity thus by changing the ecosystem pattern (Authman MMN,2008). Fish are the tertiary consumers in the aquatic food chain; hence they accumulate metals and ultimately pass them to the human beings causing several disorders. Studies show that accumulation of heavy metals in a tissue is mainly dependent on water concentrations of metals and exposure period; although some other environmental factors such as water temperature, oxygen concentration, pH, hardness, salinity, alkalinity and dissolved organic carbon may affect and play significant roles in metal's accumulation and toxicity to fish (Jitar O.,2014). Other factors that affect the levels of accumulation of heavy metal concentration are ecological needs, size and age of individuals, their life cycle, feeding habits, and the season of capture were also found to affect experimental results from the tissues (Onen SA, 2015). Metals which have high uptake and low elimination rates tend to get more accumulated more likely in the fat tissues like liver. Pollutants preferentially in their fatty tissues like liver and the effects become apparent when concentrations in such tissues attain a threshold level (Omar WA et al, 2014). Overall, metals can be classified as essential and non-essential. The nonessential metals like, aluminium (Al), cadmium (Cd), mercury (Hg), tin (Sn) and lead (Pb) have no proven biological function also known as xenobiotics or foreign elements, and their toxicity rises with increasing concentrations. Essential metals like, copper (Cu), zinc (Zn), chromium (Cr), nickel (Ni), cobalt (Co), molybdenum (Mo) and iron (Fe) are of greater importance (Sfakianakis DG,2015).

Lead is one of the most known toxic heavy metals and its derivatives are included in the grey list of international conventions (Taylor et al., 1985). Lead is not required by any living organism hence it is one of the limited class of purely toxic elements. The largest source of environmental contamination of lead is use of paints which contains lead as there are no mandatory standards in its disposal. Mercury (Hg) and its compounds have been parts of prevalent pollutants of the aquatic environment. As per the records, the main source of mercury getting release in the environment is through fungicides, especially in the organic fungicides as mercurial materials which are organic compounds of mercury. The chronic data about mercury toxicity indicated that the organic form of Hg, methylmercury ($MeHg^+$) is the most chronically toxic of the mercury compounds. Recent reports indicate lead and mercury as a pollutant causes various neurological, reproductive, immunological, gastrointestinal and histochemical changes in the animals (Abdallah et al.,2010).

Heavy metals are known to persuade oxidative stress and/ or carcinogenesis by mediating free radicals/reactive oxygen species. Oxidative stress occurs when there is an excess of free radicals, or reactive oxygen species (ROS), in the body (Javed M, 2015). Studies has shown that excessive accumulation of ROS substances will lead to cellular injury, such as damage to DNA, proteins, and lipid membranes. ROS damage has been implicated within the development of the many physiological problems, like ageing, asthma, arthritis, diabetes, cancer, inflammation, cardiovascular disorders, atherosclerosis, Down’s Syndrome, and neurodegenerative diseases. Glutathione is a key intracellular tripeptide thiol made up of of glutamic acid, cysteine, and glycine. Glutathione helps protect cells from radical damage by acting as an antioxidant. Within cells, glutathione exists in reduced (GSH) and oxidized

(GSSG) states. In healthy cells and tissue, more than 90% of the total glutathione pool is in the reduced form (GSH) while less than 10% exists in the disulphide form (GSSG). The high GSH concentration is due to the enzyme that transitions it from its oxidized state (GSSG), glutathione reductase, is essentially active and is capable of inducing upon oxidative stress. An increased GSSG-to-GSH ratio is taken into account indicative of oxidative stress. Reduced glutathione's thiol group provides reducing equivalents to other unstable ROS, which successively becomes unstable itself. This unstable GSH readily reacts with another unstable GSH to make a stable GSSG molecule. This reaction is ubiquitous since glutathione is present in high concentrations. GSSG is subsequently converted back to GSH by the action of enzyme glutathione reductase. In addition to its role in oxidative stress, glutathione also helps maintain exogenous antioxidants like vitamins C and E. Glutathione is involved with the breakdown of peroxides. It has a task in regulating the aqua fortis cycle. Glutathione has the ability of binding directly to many inorganic and organic xenobiotic (foreign chemicals) and carcinogenic compounds, such as the heavy metals mercury and arsenic. It is important to the proper function and maximum effect of the immune system. In addition, glutathione is fundamentally involved many metabolic and biochemical mechanisms like protein and prostaglandin synthesis, DNA synthesis and repair, maintenance of disulphide bonds in proteins, enzyme activation and amino acid transport across cell membranes (Mandeep Kaur,2017)

Methods and Materials

Healthy and active Adult carp Carassius auratus (Family: Cyprinid), were purchased from the local vendor, Kalyan (19.2403º N, 73.1305º E), Maharashtra, India. Auratus was acclimatized in the laboratory conditions as per the OECD, EPA guidelines. The fish were placed in large tanks with aerated tap water. Fish were acclimatized for 2 weeks prior to the experiment under a natural photoperiod of 12-12 h. The tap water used for fish aquaria and later during experiment had a pH value of 7±0.2 and a total hardness of 20 mg caco3/L was renewed every day maintaining the temperature between the physiological tolerable limits of 25-30℃. Other physical and chemical parameters like dissolved oxygen, dissolved carbon dioxide, salinity was analysed using standard protocol (APHA)

Adult Carp (7 in each aquarium) of 20 ± 0.5 gms weight irrespective of their gender were selected for the exposure. Further, acclimatized to the laboratory conditions in 20L glass aquaria (39"X39") containing dechlorinated tap water of the quality used in the test. The fish were fed regularly with fish food pellets available commercially during acclimatization and test periods, but was stopped one day prior to exposure to the test medium for acute toxicity test only. The LC50 with 95% confidence limits for Lead were estimated for 96 h by probity analysis (Finney, 1971). The fish were then exposed to analytical grade lead acetate and mercuric chloride solutions at the concentration ten times lower (1/10th value = 2.958mgl-1) and (1/10th value =0.465mgl-1) than the recorded LC50 value (29.58 mgl-1) and LC50 value (4.65mgl-1) respectively. The fish were exposed to these pollutants for two different durations of 7 and 21 and a recovery group. The control set was maintained separately.

Experimental Group

Group 1: Three sets each containing 7 fishes (control)
Group 2 A: Three set each containing 7 fishes (mercury treated)
B: Three set each containing 7 fishes (recovery set)
Group 3 A: Three set each containing 7 fishes (lead treated)
B: Three set each containing 7 fishes (recovery set)

Lipid Peroxidation Assay:

LPO was estimated by a TBARS (thiobarbituric acid-reactive substances) assay, performed by malondialdehyde (MDA) reaction with 2-thiobarbituric acid (TBA). Homogenate (0.1ml) was added in 0.1ml each of 150mmtris-hcl (ph-7.1), 1.5mm ascorbic acid and 1.0mm ferrous sulphate in a final volume of 1ml and incubated at 37°C for 15min. To this, 1ml of 10% trichloroacetic acid (TCA) and 2ml of 0.375% thiobarbituric acid were added & kept in boiling water bath for 15min. The contents were centrifuged at 3000rpm for 10min and optical density was measured by at 532nm (Mandeep Kaur,2017).

Assay of Glutathione reductase activity (E.C 1.6.4.2)

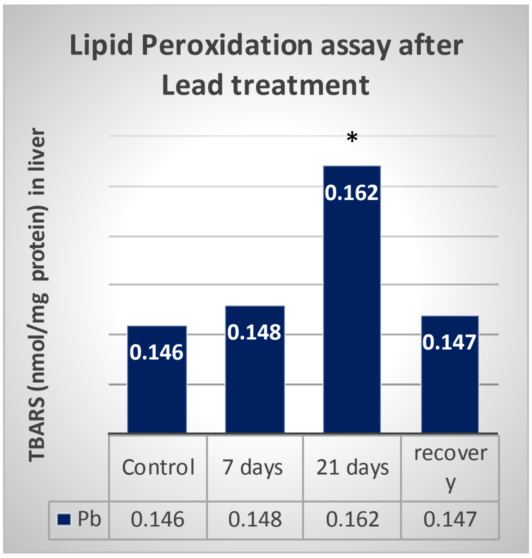
Fixed volume of tissue homogenate in phosphate buffer was mixed with a reaction volume containing 2.6ml phosphate buffer, 0.1ml EDTA and 0.1ml GSSG, 0.05ml of NADPH was added prior to assay. Decrease in the absorbance at 340nm was measured spectrophotometrically. Enzyme activity was expressed as Units/mg protein (Aniladevi Kunjamma K P,2008)

Results:

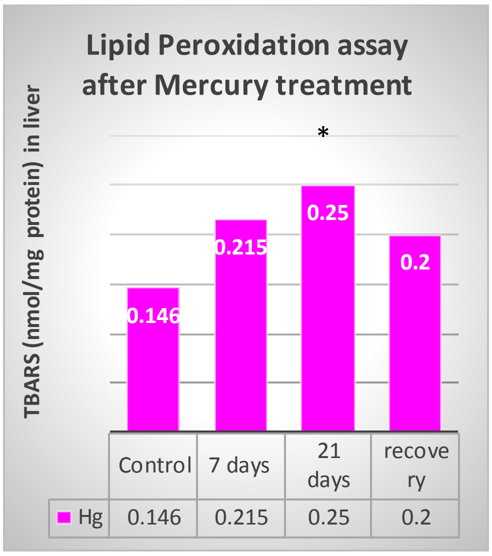
Lipid peroxidation in liver tissue was expressed as MDA in the form of TBARS (nmol/mg protein). It was reported that the rate of lipid peroxidation showed insignificant rise in 7 days treatment group over their control counterpart. Significant rise in the rate of lipid peroxidation was observed in 21 days treatment group. The results obtained showed similar traits for the lead as well mercury treatments. (Graph 1 & 2)

When the lipid peroxidation rate due to lead treatment was compared with mercury treatment, a significant rise was observed in 7 as well as 21 days treatment groups. In recovery set, the rate was noticed to be lower but the reduction was non-significant. (Graph 3).

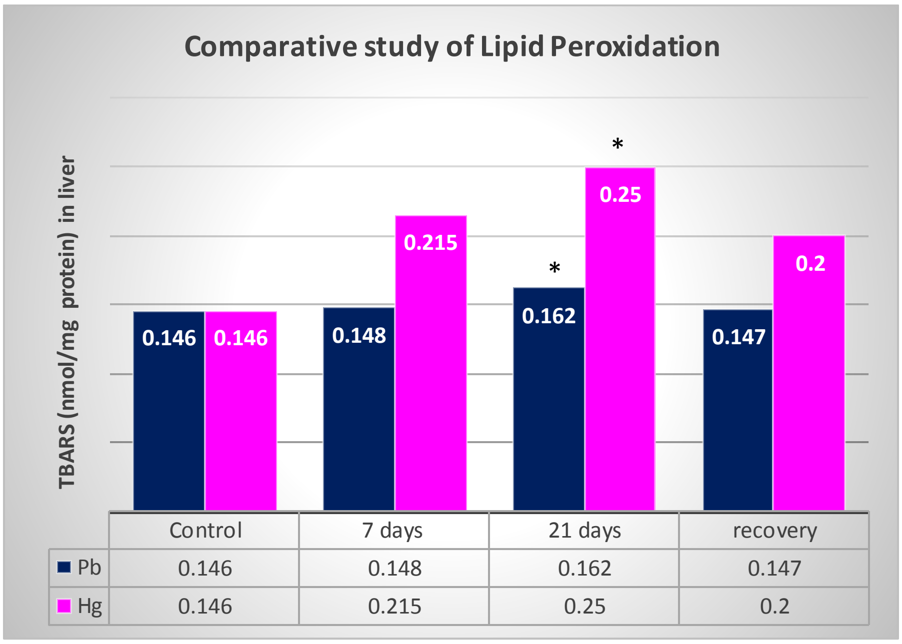
The levels of reduced Glutathione (GSH) were found to be non-significantly low in 7 days treatment group their inter-comparisons pointed at higher toxicity induced by Mercury as it seen that the levels of reduced Glutathione were significantly low in mercury treated fish over lead treated once. These results were consistent for all the treatment groups. Levels of reduced Glutathione in recovery set were found close to the control values (Graph 4, 5 and 6)



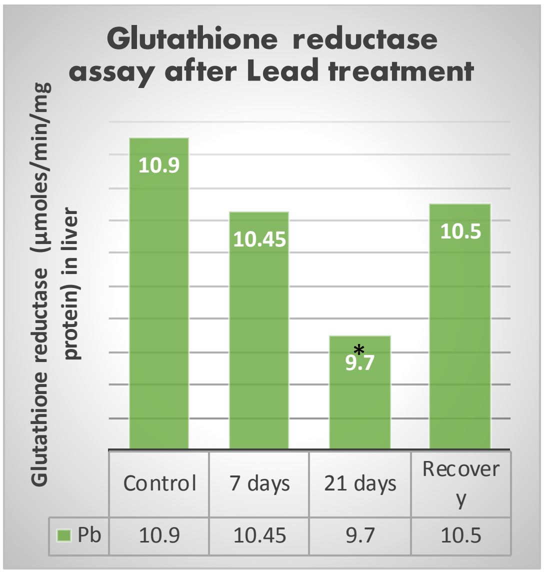
Graph 1: significance increase p≤0.005

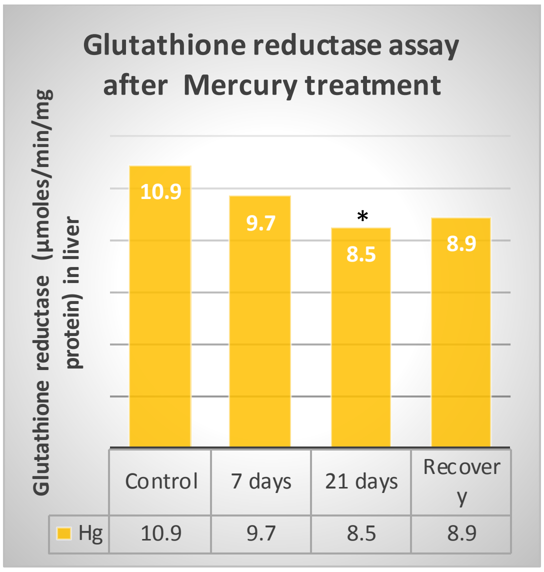


Graph 2: significance increase p≤0.005



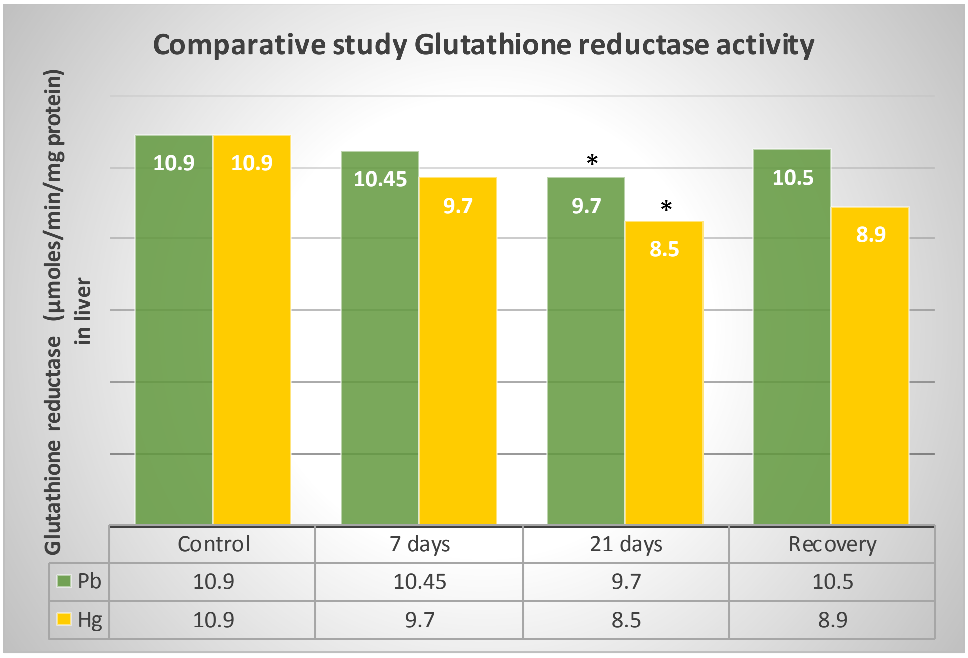
Graph 3: significance increase p≤0.005





Graph 4: significance increase p≤0.005

Graph 5: significance increase p≤0.005



Graph 6: significance increase p≤0.005

Discussion

Heavy metals of nearly all types find their ways into the environment due to several anthropogenic activities. These metals when cross their threshold concentrations, turn toxic. The toxicity assessment for the metals has been a popular field of research not only in the past but even today. Histopathological studies, Antioxidant studies, Molecular assessment, Xenobiotic studies are available for the toxicity assessment of the heavy metals.

Rate of lipid peroxidation in the form of MDA expressed as TBARS (nmol/mg protein) was determined in the past for toxicity assessment lead and mercury using – as a model. (ref). The study reported higher rate of lipid peroxidation causing tissue damage due to the two heavy metals mentioned above and also used in the current investigation.

Rate of Lipid peroxidation was found to be higher in the present studies under lead as well as mercury toxicity in time dependent manner that is the LPO rate were found to be low in 7 days treatment group then the 14 days treatment group which were in turn lower than the 21 days treatment group.

Most of the reports published in the past on the toxicity effects of Mercury and Lead are indicative of higher toxicity by mercury than any other heavy metals (Shahid Mahboob, 2013). In the present investigation similar results are seen when rate of LPO induced by mercury was compared with lead.

Reduced form of Glutathione (GSH) helps in quenching the free radicals generated during LPO. Production of GSH is facilitated by Glutathione reductase (GR). Thus, it is significant to record GR activity while studying the toxic effects of any chemical, pesticides or even heavy metals.

In the present investigation reduction in GR activity suggested the use of higher amount of GSH to counter the effects of lead and mercury toxicity in liver tissue. The effects were found to be time dependent as significant reduction in GR activity was reported in 21 days treatment group over seven- and 14-days treatment groups. When the GR activity of mercury treated samples was compared with the lead treated samples it was found that there is significant reduction in GR activity due to the mercury treatment than the lead treatment. Research reports published previously also suggested similar reduction in GR activities under mercury and lead toxicity.

Conclusion

Results obtained in the present investigations clearly suggested that both the heavy metals which were lead and mercury are capable of causing lipid peroxidation and generation of free radicles. Reduced activity of GR as reported in this investigation provides clear evidence of generation of free radicles due to lipid peroxidation of liver tissue caused due to the two heavy metals under consideration.

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Lipid Peroxidation Studies an Oxidative Stress Induced by Pyrethroid and Organophosphate Pesticides in Fish

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Abstract

Organophosphate and pyrethroid pesticides are used worldwide to protect the food crops from insects and pests. Though these pesticides are having a positive effect on food productivity it has negative consequences too. Excessive use of pesticides has a toxic effect on environment as well as non-target organisms like fish. Organophosphate such as chlorpyrifos and pyrethroid cypermethrin are known to cause high toxicity and bioaccumulation in non-target organisms. Pyrethroid pesticides have been applied to agriculture and aquaculture since 1970s to replace traditional organochlorine pesticides. A fish-specific organ such as the gills and their late metabolic action against these pesticides makes fish highly susceptible to the toxicity of pesticides. Oxidative stress plays an important role in the neurological, reproductive, and developmental toxicity caused by pyrethroids and organophosphates. Lipid peroxidation is the oxidative degradation of lipids in which, free radicals "steal" electrons from the lipids in cell membranes, resulting in cell damage. Fish exposed to cypermethrin and chlorpyrifos for 7, 14 and 21 days were studied for the oxidative damage induced in gills and an elevated lipid peroxidation was reported and expressed as (TBARS) (nmol/mg protein) as the exposure time increased.

Keywords

Lipid peroxidation, Cypermethrin, Chlorpyrifos, Oxidative stress.

Introduction

The chemical substances called pesticides are being used since decades for industrial, household, commercial as well as agricultural purposes. Pesticides have helped mankind to overcome many of their problems caused by pest (Barbhuiya Hasina Begum and Dey Mithra 2015). People today are aware of the ill effects associated with excessive use of these chemical pesticides. People are now more concerned about the non-target organisms and environmental damage caused due to the indiscriminate use of such chemical substances. Organophosphates are the group of chemical pesticides widely used across the globe. Chlorpyrifos (O, O-diethyl O-3, 5, 6-trichloropyridin-2-yl phosphorothioate) is a well-known broad spectrum organophosphate insecticide. It brings about inhibition of acetylcholinesterase enzyme present in the synapse leading to severe morbidity, loss of balance and even death. Another such widely used pesticide is pyrethroid. Cypermethrin a synthetically prepared pyrethroid insecticide is a synthetic chemical similar to the pyrethrins in pyrethrum extract which comes from the chrysanthemum plant.

All such chemical substances are posing a threat to the environment and other lifeforms. These chemicals ultimately enter and disturb the biological food chain. Fishes are the one of the best examples of being a non-target organism getting greatly affected because of chemical pollutants like pesticides.

Though oxidative stress is an inevitable component of aerobic life, in the healthy aerobic organism, a balance between the reactive oxygen species (ROS) production and the system to protect cells from ROS exists. Ascendancy of the ROS production results in defects that may bring about damages to cells or organisms or may cause their death. This imbalance is known as oxidative stress (Davies, 1995). The generation of ROS arises by many mechanisms in an organism. Physiological conditions, environmental pollution, pesticides, heavy metals, certain endogenous factors etc can stimulate generation of ROS. ROS may also play a positive role in the organism especially during the phagocytic activities of neutrophils and macrophages (Babior, 2000). Upon stimulation (e.g., From opsonized bacteria), these cells increase O2 consumption and this is referred to as “the respiratory burst” (Di Giulio & Meyer, 2008). Processes which produce oxidative stress in aquatic organisms and mammals are similar. Many xenobiotics, such as pesticides, can induce the production of reactive oxygen species by several biochemical mechanisms like impairment of membrane-bound electron transport (e.g. Mitochondrial, microsomal electron transport) and subsequent accumulation of reduced intermediates (Stolze & Nohl, 1994), redox cycling, photosensitization (Di Giulio & Meyer, 2008), facilitation of Fenton reaction, inactivation of antioxidant enzymes (Kono & Fridovich, 1983) and depletion of free radical scavengers (Winston & Di Giulio 1991).

Lipid peroxidation being one of the important biomarkers of oxidative stress in toxicity studies is a complex process known to occur in plants as well as in animals. It involves formation and propagation of lipid radicals mediated via uptake of oxygen, rearrangement of double bonds in unsaturated lipids and finally destruction of membrane lipids with the production of variety of breakdown products including alcohol, ketone, alkenes, aldehyde and ethers [Fig. 1] [Dianzani and barrera 2008,]. The rate of lipid peroxidation can be measured in terms of MDA production expressed in the form of TBARS (nmol/mg protein) [Esterbauer, H. and Cheeseman, K. H., 1990].

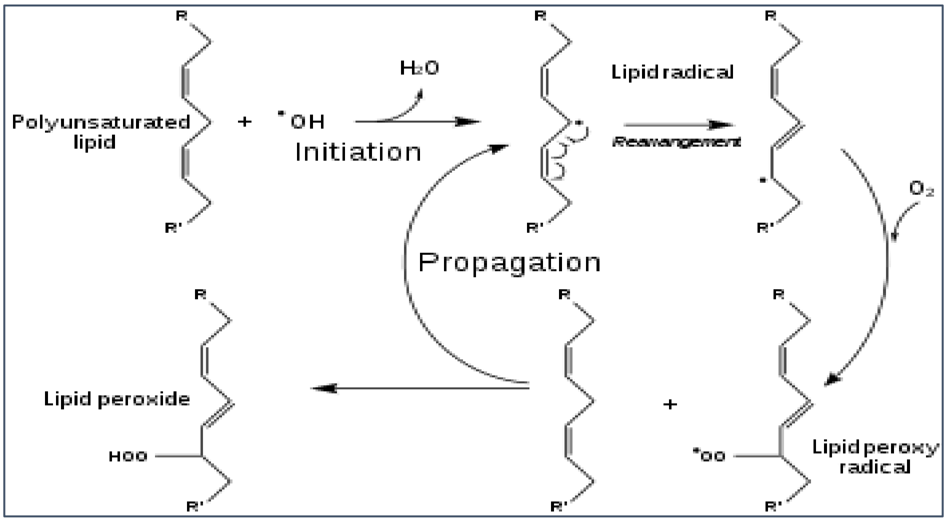


Figure.1: Lipid peroxidation pathway.

In the present study the rate of lipid peroxidation was estimated for the toxic effects caused by organophosphate and pyrethroid pesticide namely chlorpyrifos and cypermethrin viz. The effect was documented on gills of Carassius auratus commonly called goldfish.

Material and methods:

Normal potable tap water was filtered using a cotton cloth and collected in a wide and open storage tank 24 hours prior to use in a well-ventilated room with proper sunlight. This water was further transferred to the smaller tanks of 25 litres each. The tanks were labelled as follows

Group 1: Three sets each containing 7 fishes (control),
Group 2: Three set each containing 7 fishes (cypermethrin treated),
Group 3: Three set each containing 7 fishes (chlorpyrifos treated)

All the fishes were exposed to the sub lethal concentration of cypermethrin (0.025µl/l) and chlorpyrifos (0.3µl/l) and were analysed after 7, 14 and 21 days.

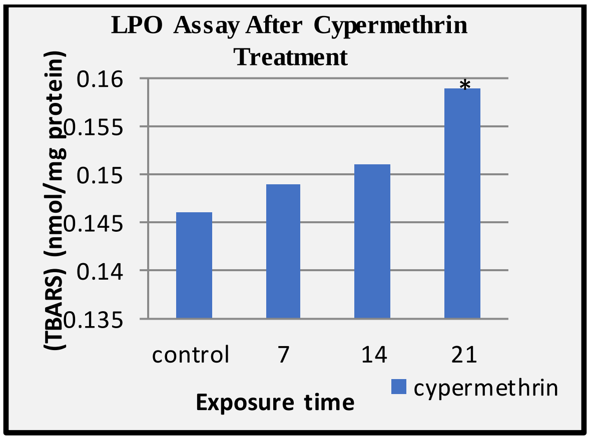
Lipid peroxidation assay:

Lipid peroxidation was assayed by measuring malondialdehyde (MDA) formation in the form of TBARS as described by (Sharma and Krishnamurthy1968). Briefly, 1.0 ml of homogenate prepared in KCl solution was incubated at 37°C for 30 min. Proteins were precipitated by adding 1 ml of 10% trichloroacetic acid (TCA) and then centrifuged at 2,000 g for 15 min. One ml of supernatant was taken as an aliquot in separate tube to which 1 ml of thiobarbituric acid reacting substances (TBA) solution was added. The tubes were kept in boiling water bath for 10 min. After cooling the tubes, the optical density was read at 535 nm.

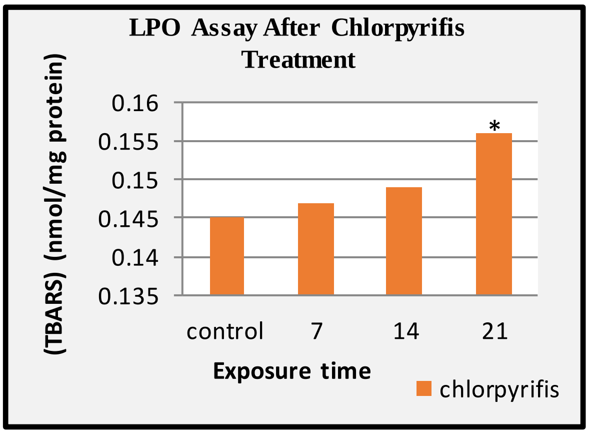
Observation and results:

Lipid peroxidation in gill tissue, expressed as MDA in the form of (TBARS) (nmol/mg protein) was found insignificantly increased in 7, 14 & 21 days over their control counterpart.

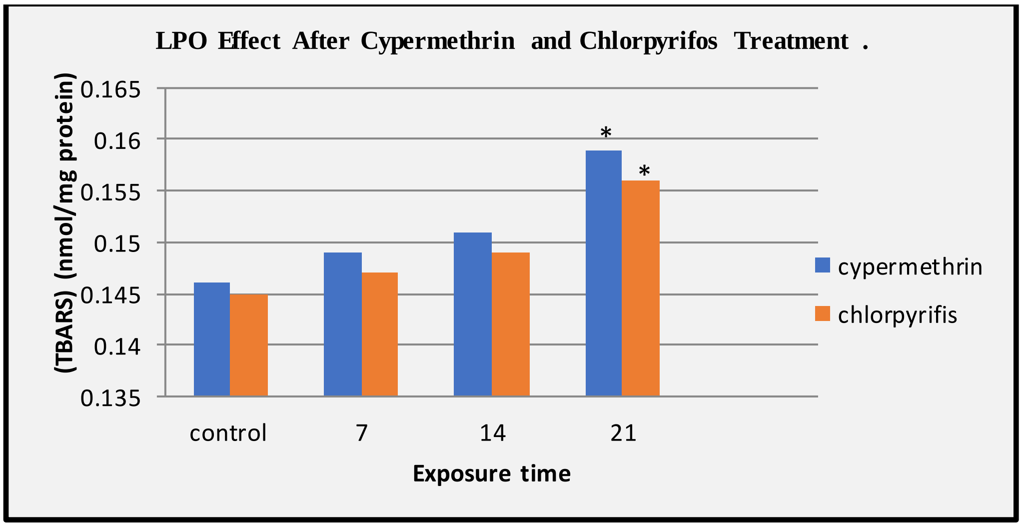
It was interesting to see a significant increase of lipid peroxidation in 21 days treatment under both the treatment regimen of pesticides (Graph 1, Graph 2). While a steady but non-significant increase is reported in 7- and 14-days treatment in cypermethrin as well as chlorpyrifos. A comparison between two pesticides indicated no significant changes in level of lipid peroxidation (Graph 3). Although it was found that the lipid peroxidation rate is non-significant in all the three groups under cypermethrin treatment regimen than chlorpyrifos.



Graph1, * - significant increase (p≤ 0.05)



Graph2, * - significant increase (p≤ 0.05)



Graph 3.,* - significant increase (p≤ 0.05)

Discussion:

Chlorpyrifos and cypermethrin are the known pesticides used for their pesticidal activities. Like all other pesticides these two candidates are also subject to considerations due to their several toxic effects caused through water pollutions. The toxic effects are especially alarming when seen in non-target animals. Oxidative stress and generation of free radicles is previously reported in non-target animals such as fish (Uner N et al 2001).

In the previous studies significantly high amount of MDA production was reported in various fishes experimentally exposed to cypermethrin (Uner et al 2001) and chlorpyrifos (Vadhva P, Hasan M 1986). The present investigation also corroborative results were obtained for both the treatment regimens.

It was found that the rate of lipid peroxidation increased with the duration of the exposure to both the pesticides. Similar results were demonstrated in earlier studies on carp, catla, carpio etc (Vadhva P, Hasan M 1986).

Conclusion:

From the foregone observations and discussion and it can be concluded that chlorpyrifos as well as cypermethrin cause membrane toxicity in the form of lipid peroxidation in time dependent manner. It can also be commented on the basis of our results that cypermethrin may release more of free radicals due to lipid peroxidation than chlorpyrifos.

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Identification and Characterization of Degradation Products of Osimertinib Mesylate Tablets by UPLC-Q-TOF and NMR Spectroscopy: Evaluation of their In-Silico toxicity for degradation products and Osimertinib.

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Abstract:

Background:

Osimertinib is a third era drug that is successful in the therapy of cancer of the lungs. The goal of this work to study the behavior of Osimertinib Mesylate (OSM) in the acid hydrolysis and characterize the resultant degradation products (dps) through UHPLC-IMS-QTOF-MS and NMR spectroscopy. Since there is no research published elsewhere on the hydrolytic degradation of OSM, therefore the present work has been completed. As the profiling of impurities is an important for the safety and effectiveness of the medications.

Keywords:

Osimertinib Mesylate (OSM), Degradation Products (dps), Acid hydrolysis of OSM, Semi-Preparative isolation, characterizations by UHPLC-IMS-QTOF-MS, NMR etc.

Methods:

There are total of four major degradation products (dps) were observed and their separation was achieved on a waters X-bridge (250 mm × 4.6 mm, 5 µm) C18 column using an HPLC-PDA gradient elution programme, with mobile phase consists of buffer (0.1% formic acid and adjusted ph 5.5 with NH_4OH) as mobile phase A and Acetonitrile as Mobile Phase B delivered at flow rate of 1.0 ml minute-1 and the detection wavelength kept as 268 nm.

Results:

Osimertinib (OSM) was found degraded significantly under acid hydrolysis stress condition. The degradation products were well resolved from OSM. The structural characterization of the all dps were carried out using UHPLC-IMS-QTOF-MS (ion mobility quadrupole time-of-fight mass spectrometer), based on the fragmentation patterns plausible structures were deduced for all dps by the appropriate mechanism. Additionally, the structures were also ascertained using NMR experiments by isolating the individual dps through semi-preparative liquid chromatography. In addition, in-silico genotoxicity assessed for all dps and along with active drug OSM by using structure activity relation (QSAR) and statistical based Multi-CASE and DEREK software's to enhance the safety of the drug.

Conclusion:

Based on the spectroscopic observation unambiguously **DP-1** is characterized as a hydroxy OSM Impurity, **DP-2** as a Des-acrylaldehyde OSM impurity, **DP-3** as a Chloro OSM impurity, and DP-4 as a OSM dimer impurity. The in-silico Genotoxicity assessment shows positive alerts for **DP-2** and **DP-3**, whereas **DP-1** and **DP-4** shows Genotoxicity negative.

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Biodiesel from Vegetables Oil and Fatty Acids

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Abstract

Biodiesel as an assortment of long-chain monoalkylic esters from fatty acids achieved from renewable resources, to bridge the gap between industrial production and demand of mankind to be used in diesel engines. Due to the increasing economic concerns and environmental awareness about the use of petroleum-derived fossil fuels. It is necessary to pay attention on natural renewable resources. Hence, in the present studies biodiesel was prepared by transesterification process from waste material. Fifty cm^3 of vegetable oil produced 70% biodiesel. Excitation of electron in biodiesel is due to absorption energy which change of quantum state of it from golden yellow colour to brown. Along with its other physical properties indicates that the decrease the amounts of greenhouse gas emissions and minimize the "carbon footprint" of agriculture.

Keywords

Agricultural wastes, Biomass, Biodiesel, Extraction, Transesterification.

Introduction

Development in the field of biofuels in general and biodiesel in particular are not new endeavours. However, the field is major concern about the increasing economic, environmental awareness and about the use of petroleum-derived fossil fuels [Mustafa Balat (2005)]. Several inexpensive and accessible bio resources and agro-industrial wastes are available for liquid and gaseous biofuels production including biodiesel, bioethanol and biogas (Esteffany de Souza Candeo et al. (2020). Production of biofuels in general and biodiesel in particular is gradually becoming a vital issue due to the rare-faction of the fossil fuels and the urgent need to decrease the amounts of greenhouse gas emissions (Madhumanti Mondal et al. (2017). It's necessary to review the articles on the bioconversion of renewable bio sources and agricultural by-products into bioethanol to get the information about biodiesel from bio resources. The main constituents of of vegetable oil and fats are triglycerides which is used in diesel engines as renewable resources. According to Sharp, et al. C.A. 1967 from natural resource biodiesel can be obtained transesterification process by blends with diesel fuel are indicated as ''Bx'', where ''x'' is the percentage of Biodiesel in the blend. B1 to B100 where B100 indicates pure Biodiesel. There are catalytic and non-catalytic methods for transesterification reactions to the prepare biodiesel from the waste materials (A.Demirbas 2005,).The diesel was analysed spectroscopically by S. Oliveira (2006);A Saliacet (2011). The reversible reaction is carried out by mixing the reactants – fatty acids, alcohol and catalyst which gives raw biodiesel and raw glycerol catalytically. The production of Biodiesel non-catalytically from vegetable Oils or animal fats by using supercritical methanol which is an alternative, cost effective, time saving process for the production of biodiesel.

Catalytic method with an alcohol transesterification reaction carried out and proposed to use in diesel engines, alone or blended with diesel oil by J. Alamu et al.2007. The properties of biodiesel vary as per the nature of raw material, geographical condition and the methodology used for the isolation and characterisation to observe the 100% renewable energy. With this background the present proposal deals with the production of biodiesel from bio resources such as vegetable oil and esters/fatty acids.

Material and methods:

Source-

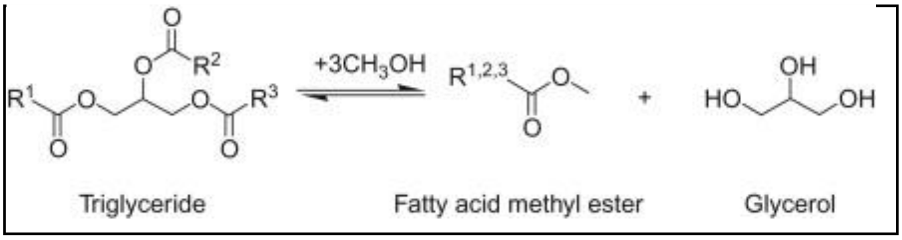
Vegetable's oil was isolated from a waste material mango seed kernel which was refined through degumming, neutralization and bleaching process using local adsorbent (activated clay) (Mahale et al, 2012),

Methods

The most common method for obtaining it is the transesterification. In this process, the triglyceride is reacted with methanol in the presence of a catalyst to produce a mixture of fatty acid methyl (or ethyl) ester, (FAME) and glycerol. The FAME are separated before to be used as biodiesel, in substitution of diesel. Following are the methods for the preparation of biodiesel

Transesterification will be carried out by using vegetable oils (50 cm^3) waste by using strong base or a strong acid as a catalyst .in the present reaction, after adding Sodium hydroxide in mango seed kernel oil, it was (50 cm^3) in a blended for 20 minute. The absorption of lye is done with by adding Ethylene glycol (200 cm^3) in sodium hydroxide at high temperature which produced sodium methoxide. Segregation of layers of biodiesel and glycerine was observed after 25 to 30 min of blending. After 10 hrs, solid glycerine was separated from biodiesel. Biodiesel was washed with water by pouring water in it.

Reactions:



Results and discussion:

In vegetable oils, higher oxygen content allows biodiesel to burn more completely. Food Industrial waste contains lipids, food residues and free fatty acids. In the present study 50 cm3 of mango seed kernel oil was taken for the process of transesterifications that produces 35 cm^3(70%) of biodiesel. The biodiesel is in laboratory scale hence its production, physical characteristic and quality may differ from the large-scale production. The physical properties are shown below-

Physical Properties of Biodiesel:			
Sr. No.	**Property**	**Physical Properties of Biodiesel**	**Inferences**
1	Yield	35cm^3 biodiesel	Pure biodiesel will thicken and cloud
2	Colour:	Golden to dark brown	Excitation of electron due to Absorption energy which change of quantum state. It exhibits more oxides ion in oil. In UV it brings the absorption band from the UV to the visible region
3	Flame test	Flash point test	Flash point test varies in each set may be depend on lubricity of oil from 700C to 92 0C
4	Boiling Point	315°C to 350°C	Main constituents is Triglyceride and how carbon are carried out in biodiesel in the FAME (fatty acid methyl (or ethyl) ester).
5	Density@15°C :	860-900 kg·m^{-3}	To observe atomicity
6	Calorific values and Thermal efficiencies	Not tested	Not tested

Interferences of Bioethanol may be varied as per reactant/biomass used in the reaction mixture because of plants are rich in sugar content, Phyto-constituents' lipids, antioxidants free fatty acids etc. That need to address before isolation of biodiesel from biomass. Yield of biodiesel depend on thermal condition used in reaction.

Global demand of Petroleum product more as compare to resources are very limited since last decade. Its cost is also high, preparation transportations may add in it. Hence, the alternative cost-effective renewable biodiesel. This small step may advance petroleum chemistry.

Conclusion:

The Biofuels prepared from vegetable oil with esterification method can be used for heating, lighting, power and transport. Transesterification reaction is cost effective time saving and economical viable reaction. It is nontoxic required less time and for washing used green solvent to observe the clear biodiesel. Yield of the biodiesel is recommendable since it is produced by natural resource. It can also use in various skin disease along with the machine and as fuels.

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An Alternative Dye; Curcumin Extraction Method and Its Application

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Abstract:

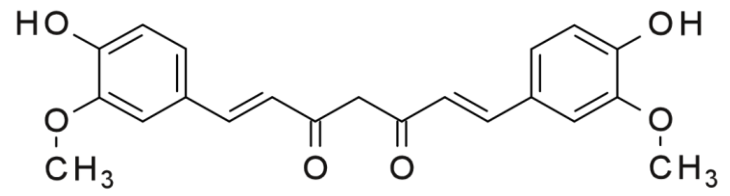
Due to eco-friendly approach of natural dyes, growing interest of researchers for various applications of it. Natural dyes contains impurities which gives tolls in the field of medical, textile, cosmetics, leather and pharmaceutical chemistry. Present study deals with extraction and purification of natural dyestuff from plant *Curcuma longa* . The dye was isolated by green solvent as well soxhlet extraction method and used dyeing of cotton fabric. The dyeing method was optimized various factors such as PH, temperature and time. Due to its fastness property and as an alternative dye to synthetic dyes, it helps environment and for human health.

Keywords:

Natural dyes ; Curcumin ; cotton Fabric

Introduction

A colour substance has affinity on which it is being applied. Curcumin is one of the natural dyes having antioxidant, anti-inflammatory properties which are isolated from *curcumin longa* (Hema Suryawanshi et, al. 2017) Turmeric is perennial herbs and source of flavouring agent used in culinary. Since synthetic dyes are carcinogenic nature, researchers paying attentions towards natural dye. Curcumin ($C_{21}H_{20}O_6$) that generate yellow to orange in colour. The research shows that the ratio of turmeric juice to mordant of 2:1 without any emulsifiers contributed the superlative colour strength and colour fastness. Curcumin antioxidant stimulates the brain, has role in Alzheimer (Pierce.1993). The yellow colour of curcumin which helps for depression mood to improve upon (Ishita C. 2004). The yellow dye produces different shades of yellow colour on the cotton fabric with different dyeing conditions and use of mordant. (Sainath Umbreen et al 2008; Agarwal, K 2009) In the present scenario, due to the excelling advantages of natural dyes, it is becoming an enticing option over synthetic dyes. Chemistry of Curcumin (Ishita C. 2004; Koren, Z.C 1995)

Curcumin	
Colour	Orange-yellow
Solubility	Insoluble in water and Soluble in alcohol
Molecular Formula	$C_{21}H_{20}O_6$
Molecular Mass	368.38 g/mol
IUPAC Name	(1E,6E)-1,7-Bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione
Melting Point	183°C (361°F, 456K)[4].

MATERIALS AND METHODS:

Materials:

Round bottom flask (1000 ml), beaker (100 ml, 200 ml), Soxhlet apparatus, aluminium vessel, curcumin roots, cotton fabric, Mixer grinder, Thermometer, Weighing balance, Burner, pH meter, Computer colour system. Ethanol, metal salts (mordants used $CuSO_4$, $FeSO_4$), glass distilled water.

Methodology

Source: **Curcuma longa**/ turmeric roots was used for dyes preparation. Washed well dried grounded in powdered form. Crude dyes used for the dyeing fibres. Morphology of curcuma longa is as follows-

Figure 1 Morphology of Curcuma longa

Extraction of Crude Dyestuff:

Curcumin powder (10g) in 500ml of ethanol was boiled at 60°C in water bath for 60 mins. After filtration, the obtained crude dyestuff was distilled using the Soxhlet apparatus at 70° C for 3-4 Hrs. The Concentred distilled solution was cooled at room temperature to observe precipitation of dye which was dried naturally.

Scouring of cotton cloth was carried out by using scouring agent. Scouring of cotton fabric is done by using scouring agents like NaOH, Na_2CO_3 etc. Which removes all the impurities present in the fabric. (Lauresen, Z 2005; Kanchana, R 2013)

Direct dyeing was carried out by common salt and Glaubers salt. Cotton fibres are soaked boiling water bath for 8-10 minutes to fix the dye on the fibre. After exhaustion the fabric is transferred to cold water bath to eradicate free dye from fabric.

OPTIMIZATION OF DYEING CONDITIONS

Cotton fabrics are dyed with the curcumin dye at liquor ratio of 1:40 (1kg of fabric in 40L of solution). For the optimization of dyeing conditions which affects the colour strength of dye,

Optimization of dyeing pH:

Dyeing procedure is carried out with 2% conc. of purified dye at pH 3 to 9.

Optimization of dyeing temperature and time

Optimization of dyeing on fibre was tested by varying temperature ranging from room temperature to 60, 70, 80, 90 & 100°C.

To observe significant colour on fibre, dyeing time was varying from 10 min to 120 min.

Optimization of dyeing concentration:

Another set of experiments is also carried out at different dye conc. ranging from 2% to 120 % to dye the cotton fibre.

Based on K/S (adsorption coefficient) values of dyed samples, the optimum dyeing PH, temperature and time taken for further study.

Evaluation of colour strength & % exhaustion:

Evaluation of colour strength of dyed fabrics are carried out by determining K/S(absorption coefficient & scattering coefficient) values using a computer colour matching system and the reflectance value (R) in visible region by means of double beam spectrophotometer.

The K/S and R values follows the Kubelka Munk theory by the equation,

$$K/S = (1-R)^2 /2R$$

The value of K/S is directly proportional to the conc. Of dye and it tells the depth of colour of dyed fabric.

% Exhaustion by UV/VIS spectrophotometer:

Degree of exhaustion is the amount of dyestuff is diffused in the fibre from the dyebath at the time of dyeing. Bye measuring the conc. Of dyebath before and after dyeing process at the wavelength 425nm, percentage of exhaustion obtained by using following formula.

$$E\% = (C1-C2 /C1) * 10$$

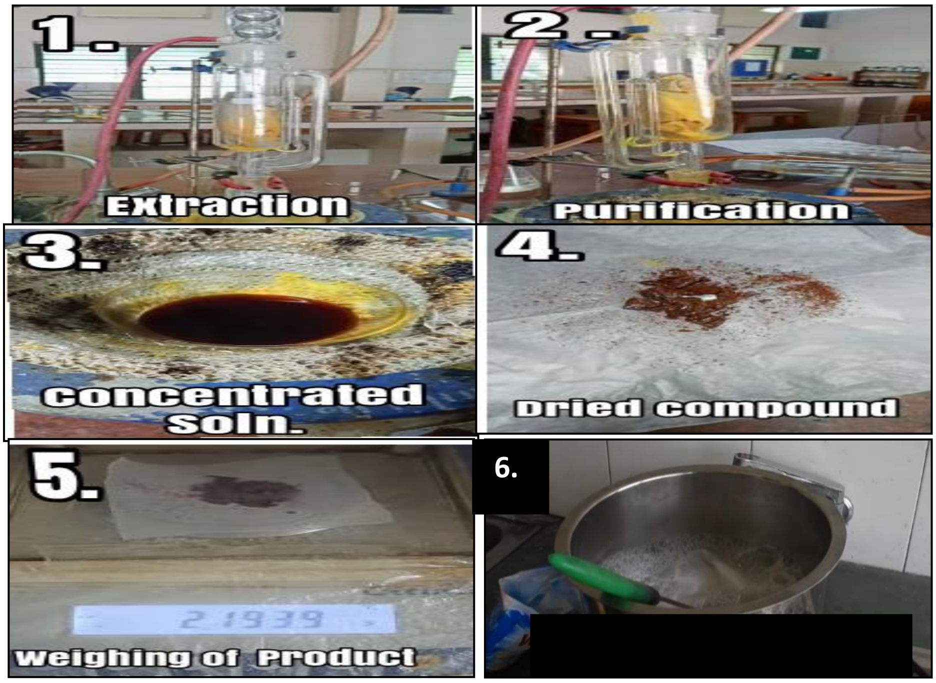
RESULT AND DISCUSSION

A natural dye, Curcumin is non-toxic, and environment friendly because it's obtained easily at home and the same chemical nature was confirmed with isolated dye in laboratory. The extraction of dyes from curcumin loga is shown in figure 2. The isolation process is well-known for its usage in food materials, pharmaceuticals and textiles, in place of their synthetic counterparts.

The optimum Coefficient of adsorption and Scattering coefficient (K/S) value was observed with 10% conc. of dye in neutral condition at 80°C. When the fabric kept in dyeing bath for 50 minutes.

The obtained dyestuff (2.180 gm) was brownish in colour. When it dissolved in alcohol and water it exhibits shades of orange yellow colour. The reflectance value of dyed fabric is measured at the wavelength 425nm and the K/S value is taken directly from the instrument. Every dye sample is analysed in the same way, the different shades of dyes shown in figure 3.

Some of the restrictions like colour yield, complexity of dyeing process, inadequate shades, amalgamation of it, physical fastness properties all are responsible for its significance because no standard profile for extraction available.



[redacted]

Figure 2 : Extraction dye from Curcuma longa

Figure 3 Dyeing of cotton fabric (picture 1 to 4); drying of cotton fabric (5 &6) and different shades of curcumin with mordant dyeing.

Conclusion

Safe, cost-effective, an alternative natural dye is easily extracted at home which was anciently used for its antioxidant and inflammatory properties. It is employed for textile dyeing along with pharmaceutical industries. The obtained yellow colour dye is curcumin is confirmed with literature survey. The fabric was dyeing with both sample homemade dye as well Soxhlet method dye. Bath dyes shown excellent strength towards the fibric. The highest degree of exhaustion of cotton fabrics, dyed with different methods, are determined by the UV/VIS Spectroscopy indicating respect to concentration, time, temperature for dyeing the cotton fabric.

Acknowledgment:

Greatly acknowledge to Lifeon Labs pvt. Ltd., Dombivli (E) given opportunity to Hrutik to carried out his project work. Dr. Anita S. Goswami-Giri and HOD, B N Bandodkar College of Science for inculcating of research aptitude

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Recycling and Quality Improvement of Laboratory Chemical Wastes

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Abstract

A chemical disposal plant was fabricated for reuse and recycle of chemical waste water from chemistry laboratory. Various physical and chemical properties of waste water collected from chemistry laboratory were studied. The properties such as ph, Turbidity, Salinity, Alkalinity, Chemical Oxygen Demand, Dissolve Oxygen, Hardness of water, Flame photometer, etc. Were studied before and after processing of waste water. The studies after processing shows that the water thus treated can be drained in nearby water bodies without affecting flora and fauna. Use of this type of chemical disposal plant as a reductive medium is receiving increased interest due to its low operation cost and maintenance.

Keywords
Water parameters, Chemical waste water treatment, 3R model, Chemical Disposal Plant.

Introduction

India is facing a water quality crisis due to haphazard urbanisation and rapid industrialization. Consequently, there is a continuous pressure water resources and increasing the unregulated discharge of contaminated waste water within the urban area. Various chemical laboratories located in different colleges and various R & D labs do drain their chemical waste water in nearby water bodies resulting in water pollution and decrease in number of aquatic animals in that water body. The best solution on this is following 3R model, i.e. Reuse, Reduce and Recycle. In the process Reduce and Recycle we can reuse water for gardening and also same water can be directly drained in main water body,

Different countries have their different centralised waste water management system. The basis of the European waste survey is the Framework Directive on Waste that is set out in Council Directives on Waste 75/442/EEC and Hazardous Waste 91/689/EEC[1]. In addition to the directives, Regulation 259/93/EEC establishes a system for controlling the movement of waste within, into and out of the European Union[2]. The Framework Directive on Waste will be revised, probably in 2008, in order to modernize, simplify and clarify where necessary, and to reinforce standards and waste prevention[3]. It seems clear that the limitations imposed by this new Directive will make it more difficult to use sludge in agriculture and that considerable investments will be needed to fulfils the new requirements[4]. The integrated Pollution Prevention and Control Directive (96/61/CE) also applies to the pulp and paper industry. It lays down measures designed to reduce or if possible, to eliminate emissions to air, water and land.

It also includes measures concerning waste, in order to achieve a high overall level of environmental protection.

In present study we are reporting a chemical waste water treatment plant i.e., Chemical disposal plant (CDP) which will help for recycling of water and also will save flora and fauna of water body where chemical waste water has drained.

Experimental details

The study is mainly divided into three parts namely; measurement of water quality parameter before treatment, treatment to water using chemical disposal plant and testing of treated water for various quality parameters.

Materials

Disodium salt of Ethylenediaminetetraacetic acid (EDTA) (MOLYCHEM Pvt. Ltd.), Anhydrous Sodium bicarbonate, (nahco3)– (LOBA Chemicals), Potassium Dichromate – (MOLYCHEM Pvt Ltd.), Manganese sulphate – (LOBA Chemicals) , Sodium Hydroxide (MOLYCHEM Pvt Ltd.), Potassium Iodide – (MOLYCHEM Pvt Ltd.), Potassium Chloride – (LOBA Chemicals), Glycerol (MOLYCHEM Pvt Ltd.), Ethyl Alcohol – (MOLYCHEM Pvt Ltd.), Barium chloride (LOBA Chemicals), Silver nitrate (LOBA Chemicals), Potassium chromate (MOLYCHEM Pvt Ltd), Sodium Thiosulphate (LOBA Chemicals), Sodium Chloride (MOLYCHEM Pvt Ltd.) Calcium Chloride (MOLYCHEM Pvt Ltd.), Eriochrome Black-T indicator (LOBA Chemicals), Phenolphthalein – (MOLYCHEM Pvt Ltd.), FERROIN – (MOLYCHEM Pvt Ltd.)

Methodology

In the beginning, the water from different outlets of chemistry laboratory of VPM’s B. N. Bandodkar College of Science, Thane was collected and further used of analysis. The first step of analysis was measurement of water quality parameter of collected water sample. Some of chemical and physical water parameter were studied and these include odour, colour, pH, COD, DO, Alkalinity, Salinity, flame photometry, etc. The detailed methodology of various methods is as follows:

pH: pH values of samples were measured using pH meter (Model: Equiptronic). The litmus paper test shows blue litmus turns red which indicates water samples are acidic in nature. Further pH= 7 buffer was used for standardization pH meter and to report exact value of pH of water sample.

Turbidity

Turbidity meter is an instrument by which we can measure how “Turbid” the collected sample is. Turbidity is the Cloudiness or Haziness of a fluid caused by large number of individual particles that are generally invisible to naked eye. Also, it is key test of water quality.

Procedure: To determine the amount of sulphate present in the water sample.

i. Prepared 100ppm sulphate stock solution by weighing 0.095 gm of K_2SO_4 in 50 ml standard measuring flask.
ii. Diluted the 5 cm^3 of water sample to 50cm^3 with distilled water. Transfer 5 cm^3 of the diluted water sample to another 50 cm3 standard measuring flask.
iii. Transferred the 0.25 cm^3 and 1.5 cm^3 of 100 ppm sulphate solution in two 50 cm^3 standard measuring flask. Add 5 cm^3 of NaCl - HCl reagent, 1cm^3 of water sample 10 cm^3 of glycerol-ethanol solution and pinch of $BaCl_2$ in each of the flask and dilute each of these solutions to 50 cm^3 with distilled water. Shake the flask well.
iv. Prepared a blank solution by taking 5cm^3 of NaCl - HCl reagent, 10 cm^3 of glycerol-ethanol solution and pinch of $BaCl_2$ solution in another 50 cm^3 standard measuring flask and dilute to 50 cm^3 with distilled water.
v. Measured the turbidance for each of the solution.

Salinity:

Salt is the Saltiness or dissolved inorganic salt content of a body of water. Substances that are dissolved in water are usually called Solutes. The typical seawater has a salinity of 35 ppt. The average density of seawater at the surface is 1.025g/ml. Salinity is either expressed in grams of salt per kilogram of water or in parts per thousand.

Procedure:

i. Diluted the water sample in standard measuring flask.
ii. Add few drops of K-chromate. Take 25 cm^3 of water sample and titrate under $AgNO_3$ till brick-red ppt.

Alkalinity:

Alkalinity is a chemical measurement of a water's ability to neutralize acids. Alkalinity is also a measure of water's buffering capacity or its ability to resist changes in ph upon the addition of acids or bases. Alkalinity is more important for Fish and Aquatic life because it protects against rapid changes.

i. Due to more Acidic water sample the result were not appeared.

Dissolved Oxygen:

Oxygen saturation is a relative measure of the concentration of oxygen that is dissolved or carried in a given medium as a proportion of the maximal concentration that can be dissolved in that medium. It can be measured with a dissolved oxygen probe such as an oxygen sensor or an optode in liquid media, usually in water.

Procedure:

i. Take one stopper bottle and fill with water sample, avoiding bubbles. Add 1 cm^3 of Winkler's A and 1 cm^3 of Winkler's B. Keep aside to settle the precipitate (3min).
ii. Add 1cm^3 of H_2SO_4 to dissolve the ppt of stopper bottle. Take 100 cm^3 yellow sample mixture and titrate it against $Na_2S_2O_3$ (0.025 N).
iii. Add starch solution and then titrate till blue colour is obtained. And take the burette reading.

Hardness of Water:

The simple definition of Hardness of Water is the amount of dissolved calcium and magnesium in the water. Hard water is high in dissolved minerals, largely Calcium and Magnesium. When hard water is heated, such as in a home water heater, solid deposits of Calcium Carbonate can form. The more Calcium and Magnesium in water, the harder the water. It is usually expressed in milligrams per litre (mg/l).

To estimate the amount of total, permanent and temporary hardness in the collected sample of water was analysed using following prodecure:

Part 1: Estimation of Total Hardness

i. 20 cm^3 of water sample is pipette out into a conical flask. Add 5 cm^3 of ammonia buffer and 2 drops of EBT indicator are added and titrated against EDTA from the burette.
ii. The end point is the change of colour from wine red to steel blue. The titration is repeated to get constant titre value.

Part 2: Estimation of Permanent Hardness

i. 100 cm^3 of water sample is pipette out into beaker and boiled for 20 min. It is then filtered to remove the precipitate formed due to the decomposition of temporary hardness producing salts.
ii. The filtrate is made up to 100 cm^3 in standard measuring flask using distilled water.
iii. 20cm^3 of the made solution is pipette out into a conical flask, 5 cm^3 ammonia buffer and 2 drops of EBT indicator are added and titrated against the EDTA.
iv. The end point is the change of colour from which wine red to steel blue. The titration is repeated to get constant titre value.

Part 3: Temporary Hardness

i. The temporary hardness is calculated from the total and permanent hardness. Temporary Hardness = Total Hardness – Permanent Hardness.

Chemical Oxygen Demand:

The chemical oxygen demand is an indicative measure of the amount of oxygen that can be consumed by reactions in a measured solution. It is commonly expressed in mass of oxygen consumed over volume of solution which in SI units is milligrams per litre. High COD is bad for aquatic organism.

Part 1: Standardization of Ferrous Ammonium Sulphate (FAS)

i. Pipette 10.0 cm^3 of 1N $K_2Cr_2O_7$ solution. Dilute to 100 cm^3 using distilled water. Pipette out 10.0 cm^3 of diluted sol in 250 cm^3 conical flask.
ii. Add 5 cm^3 of conc. Sulphuric acid. Cool the content in the flask to laboratory temp. Add 4 drop of ferroin indicator solution.
iii. Titrate against 0.1 N ferrous ammonium sulphate solution until the colour changes from blue to red. Repeat the titration till CBR is obtained.

Part 2: Determination of chemical oxygen demand:

i. Pipette out 20 cm^3 water sample in 250 cm^3 of standard measuring flask. Add approx. 400 mg of mercuric sulphate.
ii. Add 10.0 cm^3 of $K_2Cr_2O_7$ 30 cm^3 of the conc. Sulphuric acid reagent B measuring cylinder. Connect the reflux flask through the condenser and reflux for min. of 90 min at 1500C
iii. Add 80 cm^3 distilled water through condenser cool it to room temp. Dilute the resulting reflux solution to 250 cm^3 using distilled water. Pipette out 25 cm^3 of this diluted solution and titrate with standard FAS using 3drops of ferroin indicator.
iv. Endpoint is sharp blue-green to brick red. Reflux the same manner a blank with distilled water 20 cm^3 and follow the above procedure.

Flame Photometry:

A Flame Photometer is a device used in Inorganic chemical analysis to determine the concentration of certain metal ions, among them Sodium, Potassium, Lithium and Calcium. Group 1 and Group 2 metals are quite sensitive to Flame Photometry due to their low excitation energies. The principle of this is based on the measurement of the emitted light intensity when a metal is introduced into the flame.

Procedure:

i. Dilute 10 ml of the supplied stock solution of (1000 ppm) concentration to 100ml in a standard measuring flask with distilled water (100 ppm).
ii. Take six serially number 100ml standard measuring flask.
iii. Add 5, 10, 15, 20, 25 ml of 100 ppm sodium ion solution to the standard measuring flasks numbered from 1 to 5. Dilute the flask to 100 ml with distilled water.
iv. Dilute the supplied sample solution to 100 ml in a standard measuring flask (No.6).
v. Measure the emission intensity for each solution using flame photometry.
vi. Plot the graph of concentrations of solutions (in ppm) against emission intensities. This forms the calibration curve.
vii. With the help of emission intensity of the sample solution obtain the concentration of sodium from the calibration curve.

Results and Discussion

The results for various parameters are tabulated here Preliminary Test:

a) Colour- Pale Yellow

b) Smell-Fishy

Sr. No.	**Parameters**	**July/August Values**	**October/November Values**
1.	pH	4.43	2.30
2.	Turbidity	36.5	47.8
3.	Salinity	0.071 / lit	0.22 / lit
4.	Alkalinity	Due to more acidic nature of samples, we have not got results	Due to more acidic nature of samples, we have not got results
5.	Dissolved oxygen	5.2 cm^3	3.5 cm^3
6.	Hardness	60 ppm	80 ppm
7.	COD	55.68 mg/dm^3	249.6 mg/dm^3

Flame photometry						
Sr. No.	**Amount ppm**	**Reading $CaCl_2$**	**Amount Ppm**	**Reading NaCl**	**Amount ppm**	**Reading KCl**
1.	100	100	100	100	1000	100
2.	80	88	80	86	800	84
3.	60	66	60	64	600	68
4.	40	41	40	44	400	46
5.	20	25	20	24	200	24
6.	Sample	50	Sample	81	Sample	83

Table 1 depicts that collected water sample is highly acidic having very high value of hardness. The flame photometry results show presence of calcium, sodium, potassium elements in large amounts. Now the main aim of study is to recycle water sample and hence the chemical disposal plant is fabricated at large scale level having capacity of five litres. Before passing sample into chemical disposal plant the primary problems such as screening, aeration, sedimentation, filtration and disinfection were done as well-known standard methods. After these processes water was allowed to pass into chemical disposal plant. The typical setup for chemical disposal plant is shown below:

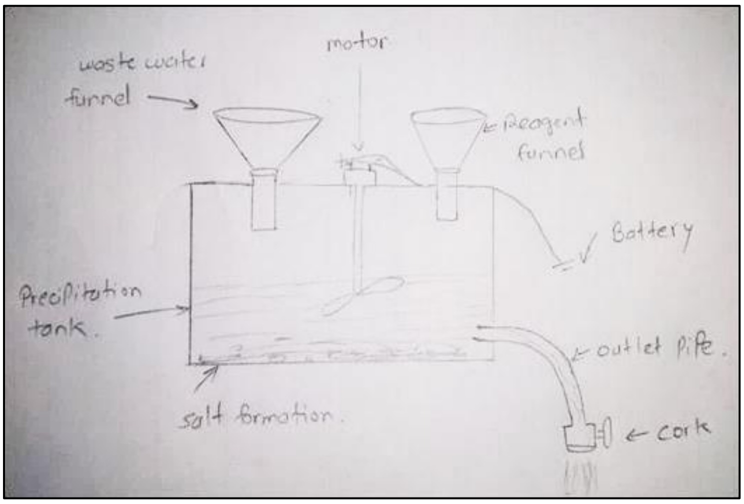

Figure 1: Chemical disposal plant

The very first treatment in chemical disposal plant was settlement of metallic elements and hence the metal which are found in flame photometer and semi micro analysis were selectively precipitated and resultant solution is centrifuge in same plant, where centrifugation setup is provided. Further to neutralise water sample the pH of water is retained by adding sodium bicarbonate. The addition of sodium bicarbonate a mild base is continued till pH of water comes to 7 i.e., Almost neutral range. After complete process the parameter of water were then tested and result are showed in table no. 2

1. Preliminary Test:
   a) Colour- Dark Yellow
   b) Smell-Fishy

Sr. No.	Parameters	Values
1.	pH	6.70
2.	Turbidity	20
3.	Hardness	40 Ppm

Conclusion

The present report aims to evaluate chemical waste management around largest chemical industrial site. Analysis of water samples is done which is collected from various labs. The results obtained from this analysis revealed that it is contaminating the water also soil pollution. The pH of water is more acidic which has adverse effect on living organism in the environment. By treating the waste water sample, we can neutralize it for that we had use some salts which adjusts the pH of water to 7. This pH adjusted water sample is then further use for house-hold purpose but not for consumption. And the salt is generated is used in laboratories; so, by this treatment on water we reuse the water without wasting it.

Acknowledgement:

Authors are very much thankful to Department of Chemistry, VPM's B. N. Bandodkar College of Science, Thane for providing necessary facilities for carrying out experiments. Authors are also thankful to Department of Zoology, VPM's B. N. Bandodkar College of Science, Thane for providing water quality parameter procedures.

References:

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Paclitaxel: Significance and Awareness

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Abstract

Paclitaxel/ Taxol is an Albumin-bound anti-neoplastic agent. It can be administered with its dosage range and with drug interaction. The present articles is focused on the monogram Paclitaxel and its route for development of the drug research. Modifications in Paclitaxel leads to the great discovery in the field of pharmaceutical chemistry.

Key Words

Antineoplastic agent, Mitotic arrest, Endophytic fungus, Albumin-bound paclitaxel.

Introduction

Paclitaxel is a well-known a chemotherapeutic agent and first member belonging to the Taxane family (Chang AE et, al. 2016). It was sold under the former generic name Taxol but its newer formulation containing Albumin-bound Paclitaxel is marketed under the brand name Abraxane. Taxol being a micro-tubule stabilizing drug and an anti-neoplastic agent has been approved by Food and Drug Administration (Zhu and Chen 2019). Paclitaxel acts as an anti-tumour drug and use to treat various types of cancers such as Ovarian, breast, lung and even AIDS-related Kaposi's sarcoma. It can also treat gastrophageal, endometrial, cervical and prostate and Head and neck cancers in addition to sarcoma, lymphoma and leukaemia. Hence, the drug is liable for blocking the cells that are existing in G2 or M phase of the cell cycle thereby causing the Mitotic arrest as such cells become unable to form a normal mitotic apparatus(Bacus, S et,al. 2001). It can be availed to the people in the form of an intravenous solution for injection. The yield of extracted paclitaxel has been increased due to the advancement in the recombination techniques and endophytic fungal have been improved. The study summarizes, the significance of paclitaxel. It is an achievement in the development of drug and having a potential impact to treat various human cancers. This monogram has been made to discuss the applications, advancement of the drug methodology, and preparation of various solutions for this drug.

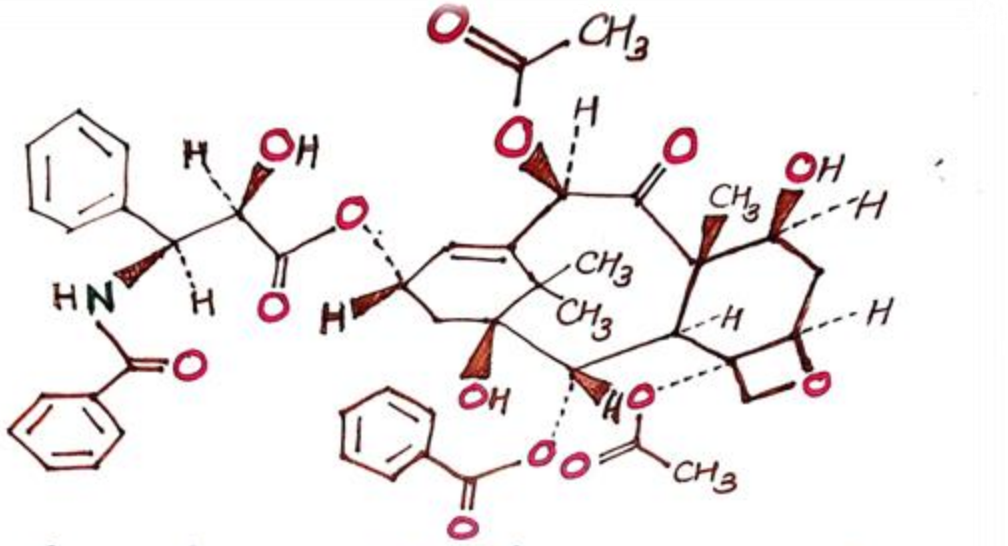
Classification of paclitaxel: Antineoplastic agents, Antimitotic agents and Antimicrotubule agents

Brands of paclitaxel: Abraxane, Onxol, formerly available as Taxol.

Chemical formula: $C_{47}H_{51}NO_{14}$

Molar mass: 85.918 g mol^{-1}

Structure of paclitaxel



5β,20 –Epoxy -1,7 β -dihydroxy - 9-oxotax-11-ene -2α, 4, 10β, -13α -tetrayl-4, 10-diacetate 2-benzoate 13-[(2R,3S)-3 (benzoylamino) -2-hydroxy -3-phenylpropanoate.

Chemical Name

[2ar-[2aα,4β,4aβ,6β,9α(Ar*,βs*),11α,1-2α,12aα,12bβ]]-β-(Benzoylamino)-α-hydroxybenzenepropanoic acid 6,12b-bis(Acetyloxy)-12-(Benzoyloxy)-2a,3,4,4a, 5,6,9,10, 11,12,12a-12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]Benz[1,2-b]Oxet-9-yl ester

Role of paclitaxel in combination therapy with other antineoplastic agents:

Paclitaxel is water insoluble, therefore it is desirable to be administered with the micelle-forming vehicle Cremophor EL which renders the drug to be soluble. But due to its unfavourable effects like hypersensitivity reactions, neurotoxic actions and alteration of pharmacokinetics of paclitaxel new delivery systems like ABI-007 have been developed for the administration along with paclitaxel. ABI-007 displays less toxicity as compared to Cremophor EL and has been considered to be more relevant for its use (Charity 2005).

Methodology: From Natural Sources:

From the plant cell cultures, large scale methods of purification have been adopted to produce high yield and highly pure Paclitaxel. The isolation has been done from the biomass of Taxus chinensis. The method of mass production of paclitaxel involves the solvent extraction, synthetic adsorbent treatment and two steps of precipitate followed by two steps of High-Performance Liquid Chromatography (HPLC) (Jin-Hyun Kim 2000). Earlier from 1967 to

1993, paclitaxel was produced from the bark of the Pacific yew, Taxus brevifolia (Gersmann 2011). The two of the scientists isolated the natural product from bark of the Western yew and determined structure and named it as “Taxol” (Wall ME 1995).

From Chemical Semi-synthesis:

In 1988, Paclitaxel was semi-synthesis from 10-deacetylbaccatin III (10-DAB) (Denis JN 1988).The drug is produced by converting the analogues or precursor such as 10-deacetylbaccatin from Taxus plants into the paclitaxel. It was carried out through asymmetric epoxidation pathway, asymmetric double hydroxylation reaction, chiral auxiliary reaction, Diels-Alder reactions, and many more (Zhu and Chen 2019).

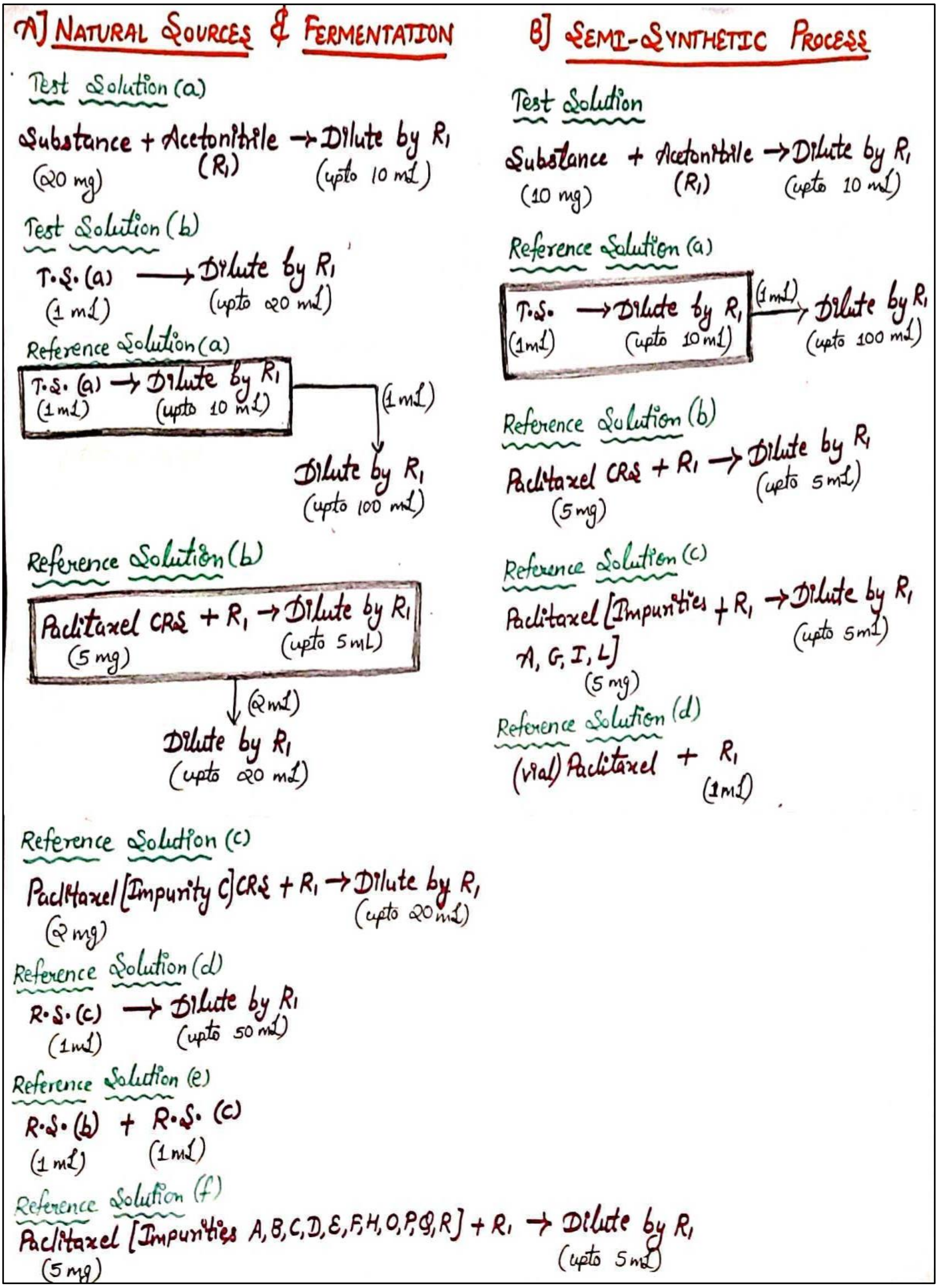
Test Solutions Preparations:

The solutions have been prepared from the different sources, which are natural sources and through fermentation and through Semi-synthetic methods. These test solutions and Reference solutions may be used for eloquent the peaks that are formed as result of chromatogram. The peaks depicts the impurity present in the paclitaxel drug that has isolated. The chart shown in handwritten format that illustrate the solutions prepared during the paclitaxel isolation. The solutions prepared during the paclitaxel isolation shown in handwritten format (Vassileva V et,al. 2008).

Paclitaxel has been resulted beneficial in the tumour immunotherapy as it improves the body immunity by producing the immune response against the tumours. It can directly kill the tumor cells such as effector T cells, dendritic cells, natural killer cells, regulatory T (Tregs) cells and macrophages (David Sarid 2006).

According to the clinical studies, Paclitaxel has also been used in the treatment of advanced (metastatic) Breast cancer. The treatment can involve the single-agent therapy, combination therapy, radiotherapy or immunomodulating drugs can be used.

The drug Paclitaxel is used to treat all types of the Cancers. Since, it has anti-tumour activity, clinical trials have been made to define the role of Texans in cancers (other than Breast cancer and ovarian cancer) such as head and neck cancers and many more. Its role is also studied in the neoadjuvant therapy (Krystyna Serkies et,al.2011).



A] NATURAL SOURCES & FERMENTATION

Test Solution (a)

Substance + Acetonitrile (R_1) → Dilute by R_1
(20 mg) (upto 10 ml)

Test Solution (b)

T.S. (a) → Dilute by R_1
(1 ml) (upto 20 ml)

Reference Solution (a)

T.S. (a) → Dilute by R_1
(1 ml) (upto 10 ml)
(1 ml) → Dilute by R_1
(upto 100 ml)

Reference Solution (b)

Paclitaxel CRS + R_1 → Dilute by R_1
(5 mg) (upto 5 mL)
(2 ml) → Dilute by R_1
(upto 20 ml)

Reference Solution (c)

Paclitaxel [Impurity C] CRS + R_1 → Dilute by R_1
(2 mg) (upto 20 ml)

Reference Solution (d)

R.S. (c) → Dilute by R_1
(1 ml) (upto 50 ml)

Reference Solution (e)

R.S. (b) + R.S. (c)
(1 ml) (1 ml)

Reference Solution (f)

Paclitaxel [Impurities A, B, C, D, E, F, H, O, P, Q, R] + R_1 → Dilute by R_1
(5 mg) (upto 5 ml)

B] SEMI-SYNTHETIC PROCESS

Test Solution

Substance + Acetonitrile (R_1) → Dilute by R_1
(10 mg) (upto 10 ml)

Reference Solution (a)

T.S. → Dilute by R_1
(1ml) (upto 10 ml)
(1 ml) → Dilute by R_1
(upto 100 ml)

Reference Solution (b)

Paclitaxel CRS + R_1 → Dilute by R_1
(5 mg) (upto 5 ml)

Reference Solution (c)

Paclitaxel [Impurities A, G, I, L] + R_1 → Dilute by R_1
(5 mg) (upto 5 ml)

Reference Solution (d)

(vial) Paclitaxel + R_1
(1 ml)

Benefits to the Society of Drug

The drug has an impressive anticancerous mechanism in which it suppresses the metastatic cell growth because it acts as a microtubule stabilizing drug. It inhibits the oncogenic cell growth by causing the mitotic arrest of the cells. Paclitaxel oil is used against the treatment of cancerous cells; even used to treat Kaposi's sarcoma. It is a type of cancer in which abnormal growth of tissue under skin is seen. Main reason of the usage of the drug is its treatment for cancer at all stages. Though in pregnancy it is safer in second and third trimester but is hazardous in first trimester due to fetal growth which results in its abnormal growth (ACS 2015). It has been hypothesized that paclitaxel can be used in the treatment of Covid-19 virus. Since its shown neoplastic and antivirus property.

Uses of Paclitaxel in various type of cancers (Esther Green et,al. 2009)-:

- Low dosage and effective doses of drugs is generally preferred to cure inflammatory diseases.
- Conventional paclitaxel and combination therapy is used for the first and second-line therapy treatment.
- The combined therapy is used along with the intravenous paclitaxel, intraperitoneal cisplatin and intraperitoneal paclitaxel for the treatment of the advanced carcinoma of the ovary.
- Non-small Cell Lung Cancer (NSCLC): Albumin-bound Paclitaxel or Conventional paclitaxel use is recommended for the First-line treatment of the advanced NSCLC.
- Epithelial cancer: Use of Combined therapy with Intravenous paclitaxel and intraperitoneal cisplatin is recommended for the initial adjuvant treatment.
- Breast Cancer: Treatment of breast cancer in patients in combination with trastuzumab is being recommended for the tumours that expresses HER2 protein. Also, Albumin-bound paclitaxel is used for the treatment.
- AIDS-related Kaposi's Sarcoma: Second-line therapy is used
- Pancreatic Cancer: Albumin-bound paclitaxel use recommended.
- Head and Neck Cancer: Active in the treatment of the metastatic squamous cell carcinoma.

Limitations of Paclitaxel

Paclitaxel has a unique mechanism of action as it acts as a mitotic spindle poison that assembles the tubulin into the microtubules and stabilizes them and blocks the depolymerization process of the microtubules which further inhibits the late G2 or M phase of the cell cycle resulting in the cell death. But it has major limitations during the administration of actual use of this drug as it is water insoluble (having concentration about ~0.3 $\mu g/mL$) and thus can be used with the other organic solvents and is formulated with polyoxyethylated castor oil i.e., Cremophor EL and dehydrated ethanol. But again, this formulation with Cremophor EL has certain side effects due to which some organic solvents are needed to be developed in order to reduce toxicity or avoid alteration of pharmacokinetics (Charity 2005). Higher dosages of Paclitaxel may lead to hair loss. Furthermore, premedication of all patients is needed to be done; if not, then it may lead to hypersensitivity of the reactions, Anaphylaxis or may be even fatal to life. Taxol cannot be used for the medication of the solid tumors having baseline neutrophil count less than 1500 cells/mm3 and also in HIV-related Kaposi's sarcoma having baseline neutrophil less than 1000 cells/mm3 its use is not recommended [14]. Inhalation of the drug in the powder form may result in the symptoms such as Dyspnea, chest pain, burning eyes, sore throat, nausea, etc. There are further side effects of this drug as such there has been no such drug which can be recognized as an ideal drug. The side effect includes Laziness, getting into depressed mindset, increase of the risk of infection. It also causes soaring of mouth due to which taste cannot be guessed. When pregnant lady is treated during the pregnancy is hazardous for her child during the first trimester as it results in its abnormal growth (ACS 2015). Higher dosage of the drug may lead to hair loss and rashes over skin. Also, it may result in the decrease of the pulse rate.

Conclusion

Study and development of the drugs have been boosted as there has been increase in the diseases even after so much development in the technology as many more diseases have been originating and multiplying within a fraction. According to the recent advances being made, the applications of this drug in tumor immunotherapy have been made. Since, paclitaxel is used for the treatment of cancer chemotherapy, it has been seen that it can increase the rate of apopstosis / the death rate of the cell. Thus, the studies also revealed the beneficial and harmful effects drugs.

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Optimized chemical synthesis of zinc oxide nanoparticles for antimicrobial activity study

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Abstract:

Zinc oxide nanoparticles were synthesized using chemical synthesis route. Effect of nature of precursor, its concentration and pH of reaction were optimized. The crystal structure of ZnO nanoparticles was conformed using X-ray diffraction pattern. It was observed that ZnO nanoparticles show hexagonal wurtzite crystal structure. The antibacterial activity of ZnO nanoparticles shows good activity against *E. coli and S. aureus bacteria.*

Keywords: ZnO nanoparticles, X-ray diffraction, antibacterial activity

Introduction:

Nanotechnology is the branch of science which deals with designing, fabrication and application of nanostructure and nanomaterials as well as study of physical and chemical properties of materials. A large number of chemicals are considered to be safe at their nano range. It is mainly due to increased specific surface area and high reactivity of the nano-materials. The large surface areas ensure an increased range of probable interaction of material with bio-organic present on viable cell surface. The oxide such as zinc oxide (ZnO), magnesium oxide (MgO), titanium oxide (TiO_2) and silicon dioxide (SiO_2) has selective toxicity to biological system suggest their potential application as therapeutics, diagnostics, surgical devices and nano-medicine based antimicrobial agents.

Metal oxides play an important role in many areas of chemistry, physics and materials science. The different properties of metal oxide enable the numerous applications in fabrication of microelectronic circuit sensors, fuel cells, coating against corrosion and as catalysts. ZnO nanoparticles (NPs) could be easily grown, environment friendly and it has various applications. It is suitable for industrial, technical and medical applications. The properties of ZnO NPs are depend upon their morphology and thus have been subject of study by many researchers.

Karam et al. [1] conducted an experiment on TiO_2 coated ZnO nano crystal as surface active material. Rochman et al., [2] explained the synthesis of ZnO nanoparticles made by sol-gel method. Datta et al., [3] studied to check the potential of *Parthenium hysterophorus* leaves extracts for the extraction of zinc oxide nanoparticles for their anti- microbial properties.

Sutrodhar et al., [4] study used green synthesis of zinc oxide nanoparticles by thermal method and under micro-wave radiation using aqueous extract of tomatoes as non-toxic and also nature-friendly reducing material for photovoltaic application. Mohan et al., [5] prepared zinc oxide nanoparticles using conventional process and the preparation using surfactant. Mclaren et al., [6] illustrated the photolytic activity of ZnO crystals and states that it would be better to deduce the specific photo-catalytic activity of a particular crystallographic plane.

The main aim of ZnO NPs synthesis is to study the antibacterial activity on gram positive and gram-negative bacteria. This property of ZnO nanoparticles is because of reduced size and enhanced particle reactivity. Human quest for innovation, finding solution of problem and upgrading the industrial yields with energy efficient and cost-effective materials has opened the avenue of nanotechnology. Among the variety of NPs, zinc oxides NPs have advantage because of extra-ordinary physical and chemical properties. It is one of cheap material in cosmetic industry, nano fertilizer and electrical device and also suitable agent for bio-imaging and target drug delivery and excellent sensor for detecting ecological pollution. A variety of synthetic techniques are used for the synthesis of zinc oxide NPs. These techniques broadly can be divided into three types, that is chemical, biological and physical methods. Nowadays, ZnO NPs have been widely investigated for plant protection product, fertilizers, soil improvement, water purification and many others. Antimicrobial active packaging is a new generation of nano-food packaging based on metal nanocomposites which are made up of ZnO NPs polymer films.

Experimental details

Materials:

Zinc acetate dihydrate $Zn(CH_3COO)_2.2H_2O$ (S-D-Fine chemicals), Zinc nitrate hexahydrate $Zn(NO_3)_2.6H_2O$ (S-D-Fine chemicals) and sodium hydroxide (NaOH) (S-D-Fine chemicals) were used as precursor for the formation of zinc oxide NPs.

Methodology for Synthesis of Zinc oxide nanoparticles

In order to synthesize ZnO nanoparticles, different preparative parameters such as nature of precursor, pH of solution, concentration of precursors, etc. were optimized in the beginning of experimental setup. ZnO NPs have been successfully synthesized using two different precursors namely Zinc nitrate hexahydrate and Zinc acetate dihydrate. Those nanoparticles which were synthesized from $Zn(NO_3)_2.6H_2O$ were named as ZnO-1 and that from $Zn(CH_3COO)_2.2H_2O$ were named as ZnO-2. The detailed methodology for synthesis of these materials is as follows:

Synthesis of ZnO-1 nanoparticles from Zinc nitrate hexahydrate ($Zn(NO_3)_2.6H_2O$)

Zinc nitrate hexahydrate ($Zn(NO_3)_2.6H_2O$) and sodium hydroxide (NaOH) each were dissolved separately in distilled water to form desired concentration of 0.1M in 1:1 ($Zn(NO_3)_2.6H_2O$: NaOH) ratio. The zinc nitrate hexahydrate was slowly added drop-wise to NaOH solution which is placed on magnetic stirrer and vigorous stirring at room temperature result in formation of transparent white solution. This transparent white solution kept overnight for settlement and crystal growth. After that excess of water is decanted from the reaction vessel and the precipitate is placed in oven at 110^0C for 3 hours.

Synthesis of ZnO-2 from Zinc acetate dihydrate ($Zn(CH_3COO)_2.2H_2O$)

Zinc acetate dihydrate ($Zn(CH_3COO)_2.2H_2O$) and sodium hydroxide (NaOH) were dissolved separately in distilled water to form liquid media of desired concentration of 0.1M in 1:2 ($Zn(CH_3COO)_2.2H_2O$: NaOH). The Zinc acetate was slowly added to NaOH solution which was placed on magnetic stirrer. Vigorous stirring at room temperature lead to formation transparent white precipitate. This reaction vessel is placed for overnight settlement and crystal growth. After that excess of transparent solution was decanted and reaction vessel is placed in oven at 110^0C for 3 hours.

In both the methods, the preparative parameters mentioned are optimized preparative parameters. The schematic of experimental setup is shown in figure 1.

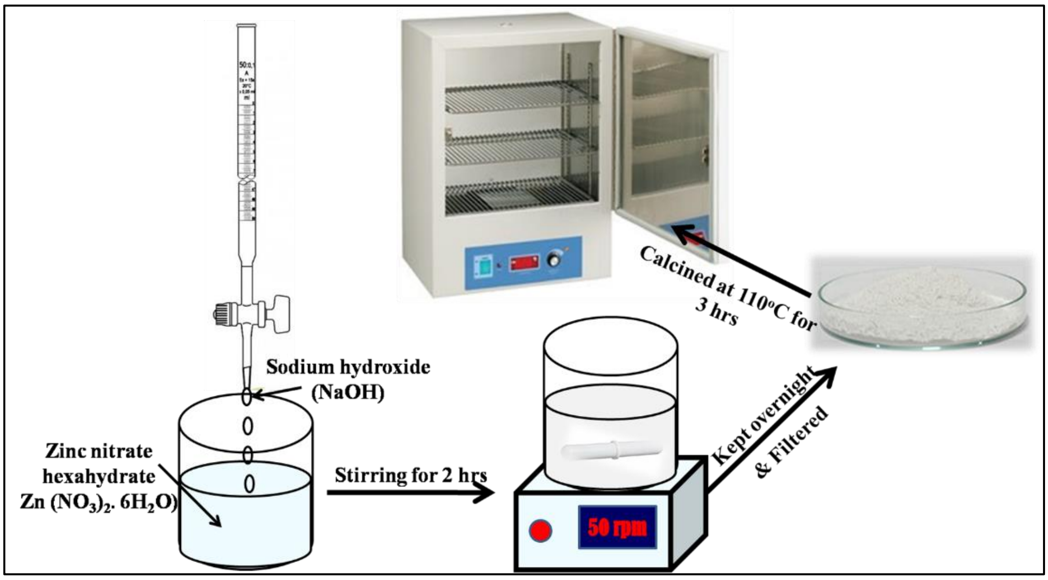


Figure 1: Experimental setup for synthesis of ZnO nanoparticles.

Results and Discussion:

Reaction mechanism of Zinc oxide nanoparticles:

a. ZnO-1 nanoparticles

The growth of ZnO nanoparticles can be controlled through the following chemical reaction:

$Zn(NO_3)_2.6H_2O + NaOH \rightarrow Zn(OH)_2 + 2NaNO_3 + 6H_2O$ ....(1)

$Zn(OH)_2 \rightarrow ZnO + H_2O$ ....(2)

b. ZnO-2 nanoparticles:

The reaction for synthesis of ZnO-2 can be controlled in following way:

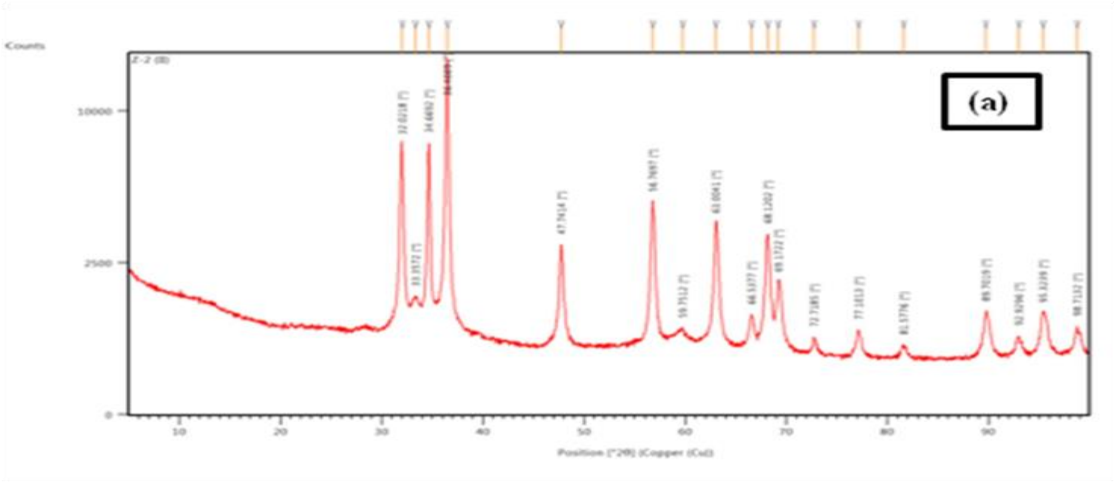
$Zn(CH_3COO)_2.2H_2O + 2NaOH \rightarrow Zn(OH)_2 + 2CH_3COONa + 2H_2O$ ....(3)

$Zn(OH)_2 \rightarrow ZnO + H_2O$ ....(4)

The formation of ZnO NPs was complex process and mostly considered to main step 1 as precipitation or formation of hydroxide and step 2 as conversion of zinc hydroxide to zinc oxide.

1.2.X-ray diffraction studies:

X-ray diffraction pattern of ZnO NP powder was investigated using XRD (Rigaku, D/MAX Uitima Japan) using Cu Kα radiation (λ = 1.54A°) in the 2θ in the range 10° to 90°. X-ray diffraction pattern of ZnO NPs is shown in figure 2.



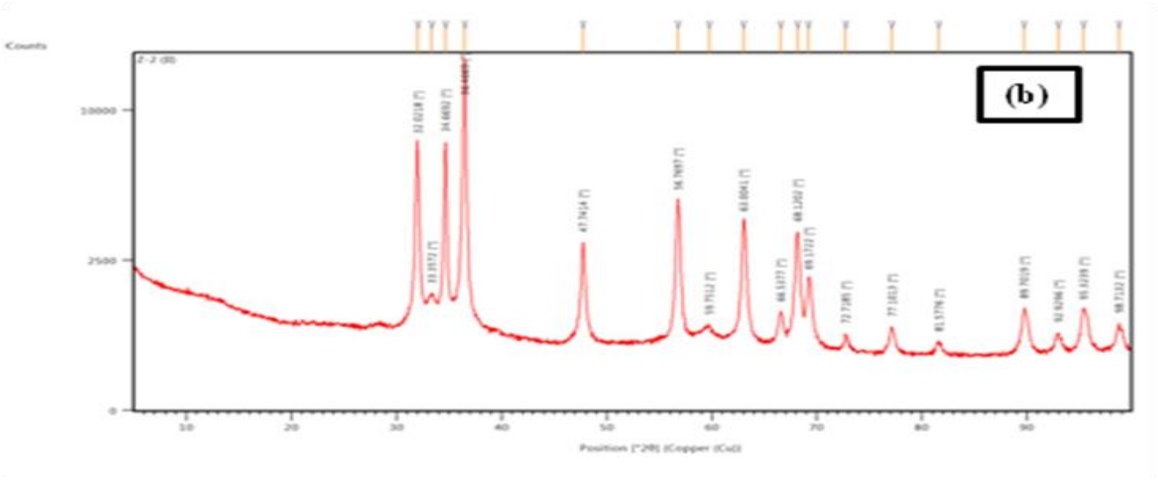


Figure 2: X-ray diffraction pattern of ZnO NPs (a):ZnO NPs using zinc acetate and (b) ZnO NP using zinc nitrate precursors.

All diffraction peaks obtained well matches with the hexagonal wurtzite crystal structure [6] of ZnO (JCPDS card no. 80-0078). The crystallite size of ZnO NPs is determined using well known Debye Scherrer formula for the prominent diffraction peak (002) and is found to be 37 nm and 24 nm for ZnO- 1 and ZnO- 2 nanoparticles respectively.

$$D = 0.94\, \lambda / \beta \cos\theta \qquad \text{......(5)}$$

where D is crystallite size, λ is wavelength of X-ray used, β is full width at half maximum (FWHM) for intense peak and θ is Bragg's angle.

1.3.Antibacterial activity:

In order to examine the antibacterial activity of the ZnO NPs on microorganism, ZnO NPs were suspended in sterile normal saline water and constantly stirring until a concentration of 1000mg/ml. Further to distribute NPS properly ZnO NP solution was sonicated for 2 hrs. To study the antibacterial activity of ZnO NPs was studied against two strains of bacteria i.e. *E.coli* (gram negative) and *S.aureus* (gram positive) by cup and well method. For this culture an appropriate volume of test bacteria was inoculated in nutrient broth medium taken in petri dish and incubated for 24hrs. After that dish was removed from incubator and by the help of borer 4 well in each plate were made. ZnO nanoparticles (ZnO-1 and ZnO-2) samples of three concentrations (i.e 0.5, 1.0, 1.5 M) were prepared and sonicated for uniform solution. After sample preparation samples were loaded by micropipette in three well of dish and control (distilled water) in remaining one well. Samples loaded dish is incubated at 37^0C for 24 hours. Then its antibacterial activity was determined by zone of inhibitions.

Determination of Zone of inhibition

Various concentration of two different ZnO NPs and deionized water as control were added in the discs wells respectively. After incubation and cultivation of different target bacteria on nutrient agar, discs and wells were placed in specific area on plates. The zone of inhibition was measured after 24 hrs of incubation. The antibacterial activity of different concentration is compared with distilled water.

Figure 3 shows comparison of antibacterial activity of ZnO nanoparticles synthesized by zinc nitrate and Zinc acetate precursors against gram negative *(E. coli*) and gram positive (*S. aureus)* bacteria. It was observed that zinc oxide nanoparticles synthesized using zinc nitrate precursors show poor zone of inhibition as compared to Zinc oxide nanoparticles synthesized using zinc acetate precursors. One of reason behind this activity may be fine nature of ZnO-2 nanoparticles as compared to ZnO-1. Also, ZnO-2 nanoparticles were prepared using acetate precursors, they facilitate formation of mesoporous morphology and hence dispersion of nanoparticles is easy. Whereas ZnO-1 NPs were prepared using nitrate precursors do not produce mesoporous nanostructures as crystallinity is more in this case.

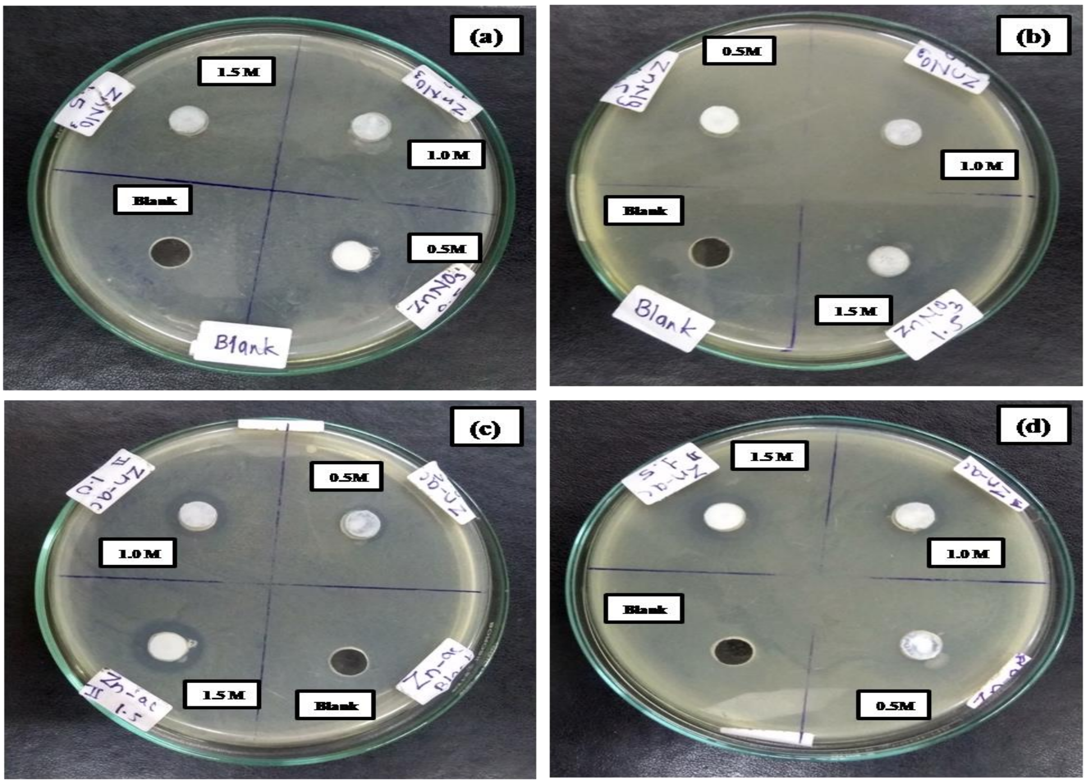


Figure 3: *Comparison of antibacterial activity of ZnO-1 and ZnO-2 nanoparticles* (a) ZnO -1 (activity against *E. coli*), (b) ZnO — 1 (activity against *S. aureus*), (c) ZnO -2 (activity against *E. coli*), (b) ZnO — 2 (activity against *S. aureus*)

Determination of minimum inhibitory concentration

After inoculation of target bacteria on nutrient agar with various concentrations of ZnO NPs, the rates of growth of bacteria were determined by counting colony forming unit (CFU) in each plate. After incubation of 24Hrs it was found that at lower concentration the growth of bacteria is slightly affected but at higher concentration of ZnO NPs solution growth of bacteria get inhibited to larger extent and clear zone of large size was obtained.

The general mechanism of action of ZnO on bacterial cell is illustrated in following schematics (figure 4).

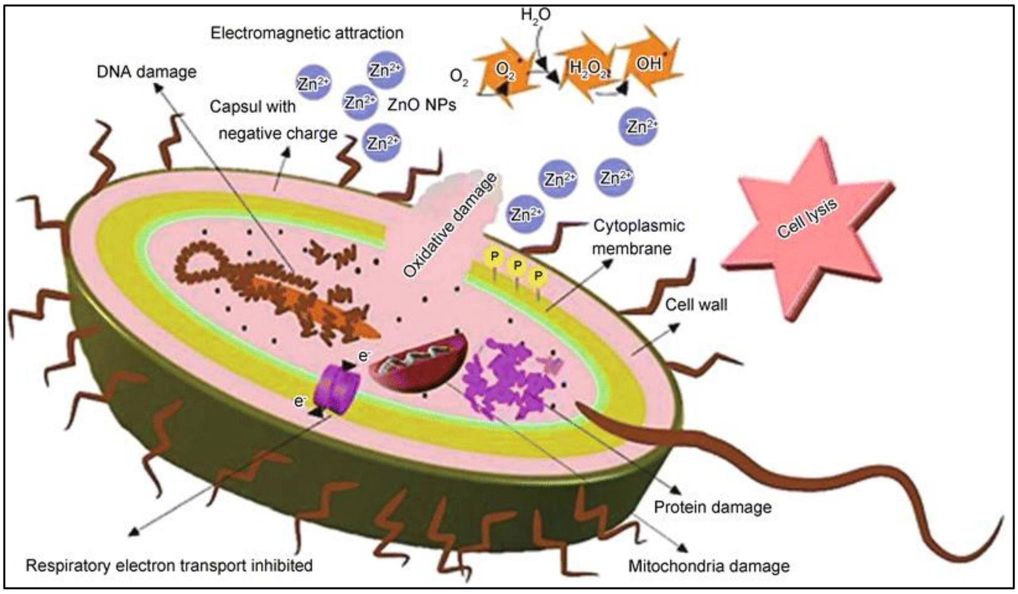


Figure 4: *Schematic illustration of action of ZnO NP on bacterial cell [7].*

In mechanism electromagnetic attraction occurs between the bacteria (with negative charge) and ZnO NPs (with positive charge) that leads to binding between them. Indeed, the ZnO NPs interact with the membrane lipids and thiol groups (-SH) of enzyme and proteins that are important for the bacterial respiration and the transport of important substance across the cell membrane and within the cell. Furthermore, ZnO NPs can penetrate inside the bacterial cell and inactivate the phosphorus- and sulfur-containing compounds such as DNA and their enzymes. Production of high levels of reactive oxygen species (ROS) such as hydrogen peroxide impacts an important role in this function. Actually, damaging of membrane, DNA and cell proteins, is as a result of ROS generation that leads to the prevention of bacterial growth and death. This process has been shown in Figure 4 schematically.

In present report the antibacterial activity of ZnO NPs were tasted by disc and well diffusion method. The presence of an inhibition zone clearly indicated the antibacterial activity of ZnO NPs. As it was also shown in study that the increasing the concentration of ZnO NPs in well and discs, the growth of inhibition has been also increased. The size of inhibition zone was different according to type of bacteria, the size nanoparticles and concentration of solution. Number of colony forming unit of *E.coli* and *S.aureus* after overnight incubation was different. This was agreement with previously published reports on antibacterial activity of ZnO which showed that minimum the concentration the growth bacteria not much affected and zone of inhibition was small but in case of higher concentration the growth of bacteria get affected to the larger extent.

Conclusion:

Zinc oxide nanoparticles were successfully synthesized by simple chemical route using zinc nitrate and zinc acetate as precursors. Both the samples of ZnO shows formation of hexagonal wurtzite crystal structure having nanocrystalline nature with crystallite size 37 nm and 24 nm respectively. Further antibacterial studies of ZnO-1 and ZnO-2 NPs show good activity. In comparison ZnO-2 shows better performance than ZnO-1 due to proper dispersion of ZnO-2 in culture medium.

Acknowledgement:

Authors are very much thankful to Department of Chemistry, VPMs B. N. Bandodkar College of Science, Thane for providing necessary facilities for carrying out experiments. Authors are also thankful to Department of Microbiology, VPMs B. N. Bandodkar College of Science, Thane for antibacterial studies, and Department of Botany, VPMs B. N. Bandodkar College of Science, Thane for providing sonication facility and to IIT, Bombay for providing XRD results.

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A Review: Comparative Study of Various Green Synthetic Methods Via Hantzsch Reaction

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Abstract:

The synthesis of aryl derivatives of dihydropyridine have importance in pharmacology since they are effective calcium antagonists. They also have antihypertensive, anti-angina, vasodilator, cardiac depressant activities, antibacterial, anticancer, anti-leishmanial, anticoagulant, anticonvulsant, anti-tubercular, antioxidant, antiulcer, and neuroprotective properties. These derivatives prepared first time by Hantzsch in 1882 after which many attempts were made to synthesise it for obtaining higher yield, purity and to find greener methods. This article will throw light on some recent trials reported for synthesis and analysis.

Keywords:

1,4 Dihydropyridine, Hantzsch reaction, Microwave synthesis, Ultrasound synthesis,

Introduction:

The aryl dihydropyridines are of great importance due to their active pharmacological and biological activities such as antihypertensive, anti-anginal and as calcium channel blockers for cardiovascular disease. Some of the drugs available in market of this class are Nicardipine, Nifedipine, Nimodipine, Felodipine, Isradipine and Amlodipine [1, 2, 3 & 4]. According to conventional method, dihydropyridine derivatives are synthesised by condensing an aldehyde with two equivalents of β-ketoester in the presence of ammonia. The previous methods of synthesis were having limitations like: longer reaction time, use of costly catalysts, higher temperature and tedious workup procedure. A remarkable variation in MCRs [5, 6, 7], developed using various ionic liquids as various Lowry-Bronsted acids, with several advantages are well documented. [8, 9 & 10]

Recently greener methods, including new catalysts, microwaves and ultrasound waves etc. were tried by the scientists for synthesis via the Hantzsch reaction. Attempts are made to make the reaction solvent free, less time consuming and convenient.

Material and Methods

Experimental details of alternative methods

A) Experiments related to microwave synthesis

1) Hydrotrope solutions are used as a medium for microwave enhanced Hantzsch Dihydropyridene ester synthesis.

Hydrotropy is the phenomenon of increasing the aqueous solubility of the substance normally insoluble or sparingly soluble in water by a third component or additive called as Hydrotrope or Hydrotropic agent [11]. The selection of solvents is important in microwave synthesis since there may be loss due to volatilisation or fire hazards etc. Use of hydrotrope is better alternative to solvents and it also has advantages like ease of isolation of products and its reusability.

The rate of heterogeneous reactions, such as hydrolysis of ester [12] oximation of cyclododecanones. Clasien-Schmidt condensation [13] etc. can be enhanced by aqueous solutions of hydrotropes .

The Hantzsch ester synthesis was carried out using 50% aqueous solution of the commercially available sodium butyl mono glycol sulphate (NaBMGS) as a solvent system, by reacting alkyl aminocrotonate with an aldehyde and alkyl acetoacetate."

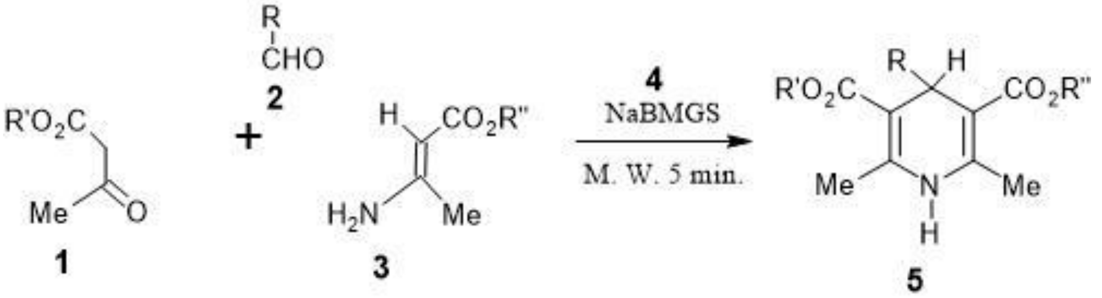


Fig.1 syntheisis of Dihydropyridene ester using NaBMGS as hydrotrope

The amount of hydrotrope solution used was just enough to dissolve the reactants. All the reactions were carried out by exposing the reactants to microwaves for 5 mins, in a glass round-bottom flask fitted with a spiral condenser containing precooled CCl_4, Better yields were obtained in nearly all reactions as compared to those previously reported, as reaction was completed in much less time, and the products could be easily isolated due to their lesser solubilities compared with the reactants.

2) Solvent-free and Catalyst-free microwave Synthesis of 1,4-Dihydropyridine Derivatives using Ammonium Bicarbonate

Advantage of ammonium bicarbonate as a source of nitrogen is that it is cheaper, less toxic and decomposes to carbon dioxide, ammonia and water vapour on heating. Initially the Hantzsch reaction of benzaldehyde, ethyl acetoacetate with various ammonium salts has been performed in solvent-free microwave conditions. The yields of diethyl-2,6-dimethyl-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate obtained in reactions carried out using different ammonium salts like Ammonium Chloride, Ammonium Sulfate, Ammonium carbonate, Ammonium bicarbonate and ammonium acetate. The maximum yield 76% and 78% was obtained using ammonium bicarbonate and ammonium acetate. In further studies, ammonium bicarbonate which has lower decomposition temperature, was chosen as the source of nitrogen. The reaction time was optimised to 25 mins as maximum yield (76%) was obtained. The Molar ratio of benzaldehyde: ethyl acetoacetate: ammonium bicarbonate giving maximum yield of 80% was 1: 2:1.5. Thus, a convenient and efficient process for the synthesis of 1,4-DHPs through solvent-free andcatalyst-free microwave induced three components coupling of aldehydes, ethyl acetoacetate or methyl acetoacetate and ammonium bicarbonate has been is simple economic and a waste-free chemical process for the synthesis of 1,4-DHPs of biological and medicinal importance.[15]

Experiments using ultrasound- Researchers attempted to use the green approach of ultrasound irradiation to further improve the known MCRs. Ultrasound enhance reaction rates by facilitating mass transfer in the microenvironment, through the process of acoustic cavitation. Cavitation occurs in an irradiated liquid and involving bubble formation, growth and impulsive collapse. The collapsing bubbles induce high temperature and pressure, in the form of hot spots with sufficient energy to facilitate chemical reactions. The Beneficial effects of ultrasound in organic synthesis is that the use of sonic waves can overcome the inconvenience of heterogeneity. A. Maquestiau determined the efficiency of montmorillonite K-10 clay supported cupric nitrate ("Claycop") for the oxidation of a larger series of Hantzsch 1,4-DHP, and to test the influence of sonication in such reactions [16]. Ultrasound offer advantages such as improved yields, short reaction times, minimal waste production, and energy savings among others, therefore it is convenient as green chemistry approach.

1) Hantzsch reactions have negative activation volumes owing to the condensation of three molecules into a single reactive intermediate and reactions with negative activation volumes are accelerated with pressure. Thus, it is well known that ultrasound irradiation [17] as well as solvophobic interactions of ionic liquids generate a microscopic internal pressure in the solvent cavity [18]. Use of TMGT for accelerating the synthesis of Hantzsch 1,4-dihydropyridines does not only show drastic improvement in yield (84–95%) over conventional thermal heating, but also shows decrease in reaction times 1.45–2.30 h) compared to classical synthesis (6–8 h). On completion of reaction, the reaction mixture can simply be washed with water, and the ionic liquid can be isolated from the product. Thus, an ultrasound-accelerated synthesis of 1,4-dihydropyridines in a simple ionic liquid, TMGT shows improvements like fast reaction, simple operation and mild reaction conditions (room temperature), high yields (84–95%), cost efficiency. One-pot synthesis of 1,4-dihydropyridines in TMGT under classical conditions and using ultrasound green aspects avoiding hazardous organic solvents, toxic catalyst, and waste (atom efficiency) [19].

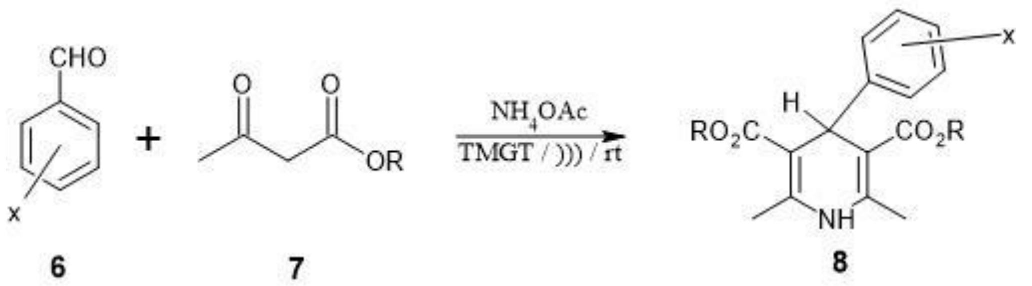


Fig.2 Preparation of 1,4-dihydropyridines using TMGT as promotor using ultrasound

2) Wang, S. demonstrated an efficient, versatile and convenient method for preparation of 1,4-DHPs by ultrasound irradiation without solvent and catalyst at room temperature. Aldehyde (1) (1 mmol), ethyl acetoacetate (2), (2.5 mmol) and ammonium acetate (1.2 mmol) were added to a 50 mL Pyrex flask. In the water bath of the ultrasonic cleaner the reaction mixture was irradiated at 28–35°C . When reaction was completed the mixture was cooled to room temperature; ice water was added and extracted with ethyl acetate. The drying of organic layer was done using anhydrous sodium sulfate and concentrated in vacuo. The crude products were purified by column chromatography on silica gel {200–300 mesh, eluted with a mixture of petroleum ether and ethyl acetate (V:V= 3:1).This improved the Hantzsch reaction due to many advantages such as mild conditions, high yields, short reaction time, easy work-up, and less toxicity. [20]

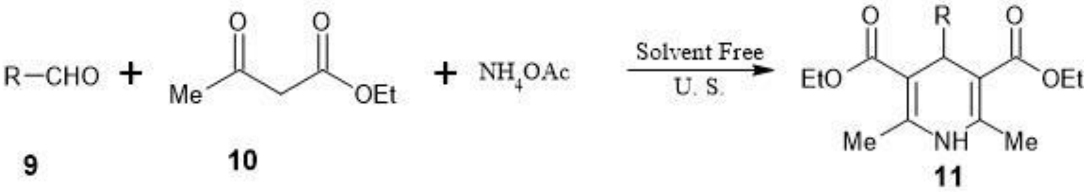


Fig.3 Title preparation of 1,4-DHPs by ultrasound irradiation without solvent and catalyst

3) One-pot, four-component catalyst free green synthesis of functionalized 1-(2-fluorophenyl)-1,4-dihydropyridins under ultrasound irradiation. The stirring of aqueous ethanol (5 mL) solution of substituted aldehyde (1.0 mmol) and malononitrile (1.1 mmol) was done at room temperature for 5 minutes. Subsequently, a solution of dimethylacetylenedicarboxylate (1.0 mmol) and 2-fluoroaniline (1.0 mmol) and aqueous ethanol (5+mL) was added to this mixture and was stirred at RT under ultrasonication for appropriate time The reaction progress was monitored by TLC. On completion of the reaction, The content was transferred into a beaker. Then, the solvent was evaporated to obtain the product in high purity. No further recrystallization was needed. [24]

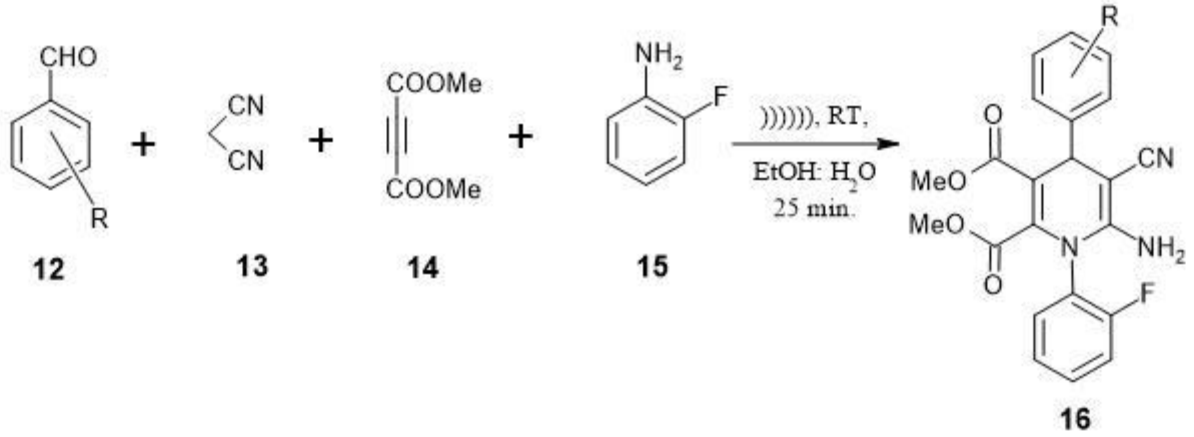


Fig.4 synthesis of functionalized 1-(2-fluorophenyl)-1,4-dihydropyridins under ultrasound irradiation

C) Other green synthetic methods

Using ionic liquid 1,4-dihydropyridine derivatives in n-butyl pyridinium tetrafluoroborate [21]. l eq. of 3-nitrobenzaldehyde, 2 eq. of methyl acetoacetate, and 1.5 eq. of ammonium acetate in ionic liquid n-butyl pyridinium tetrafluoroborate was heated at 100–110° C for 3 h and reaction mixture was cooled to room temperature. The target compound precipitated because of the very poor solubility in ionic liquid at room temperature. The resulting precipitates were isolated by filtration, washed with water to remove the water-soluble ionic liquid, and dried to give the desired product in excellent yield of 97%

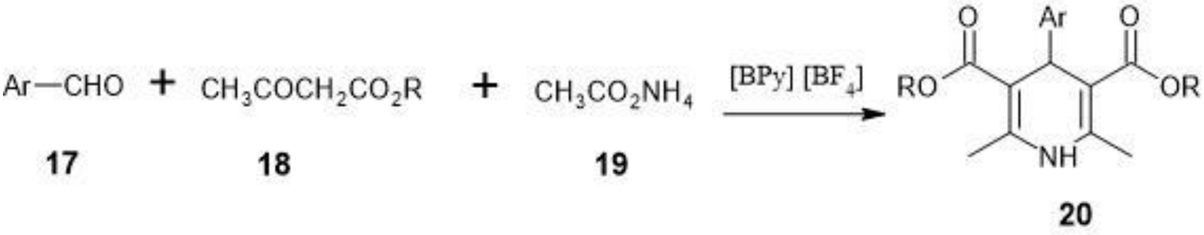


Fig.5 Synthesis of 1,4 DHP using ionic liquids.

A variety of aldehydes have been reacted with ethyl acetoacetate or methyl acetoacetate and ammonium acetate. Compared to classical synthesis, using ionic liquid as reaction media does not only provide a dramatic improvement of yields (87–97%) over conventional method but also shortens the reaction time significantly. The products were easily separated by filtration because of the poor solubility in hydrophilic [BPy][BF4] at room temperature. Therefore, the reactions avoid many problems arising from the use of volatile organic solvents (cost, handing, safety, and pollution). Another advantage of the ionic liquid is that it is recyclable as reaction medium. In view of environmentally friendly methodologies, recovery and reuse of the ionic liquid is highly preferable. The ionic liquid could be recovered easily by washing with ethyl acetate and dried over vacuum, and can be reused at least five times.

3) Synthesis in biocompatible deep eutectic solvents:

Use of ionic liquids in industrial scale has some drawbacks like high cost, environmental toxicity, requirement of high purity, etc. So, it was needed to develop alternative solvent from inexpensive, nontoxic and biodegradable components. This problem can be solved by use of Deep eutectic solvents (DES). DESs can be prepared by mixing Chlorine Chloride with amides in molar ratio 1:2 or by mixing Chlorine chloride with carboxylic acids in molar ratio 1:1. DESs proved to give better yields of desired products at optimum temperature of 60° C as compared to water as solvent or solventless conditions. The synthesis of 1,4 DHPs was done by heating substituted aldehydes with dimedone, ethylacetate and ammonium acetate in DES. This synthesis gives yields of 95% which is greater than polar and nonpolar organic solvents under similar conditions. This method has easy workup procedure as compared to products for DESs as they can be easily washed with water proving their biocompability. The DESs also gave excellent recyclability without loss of activity upto 5 cycles [22]

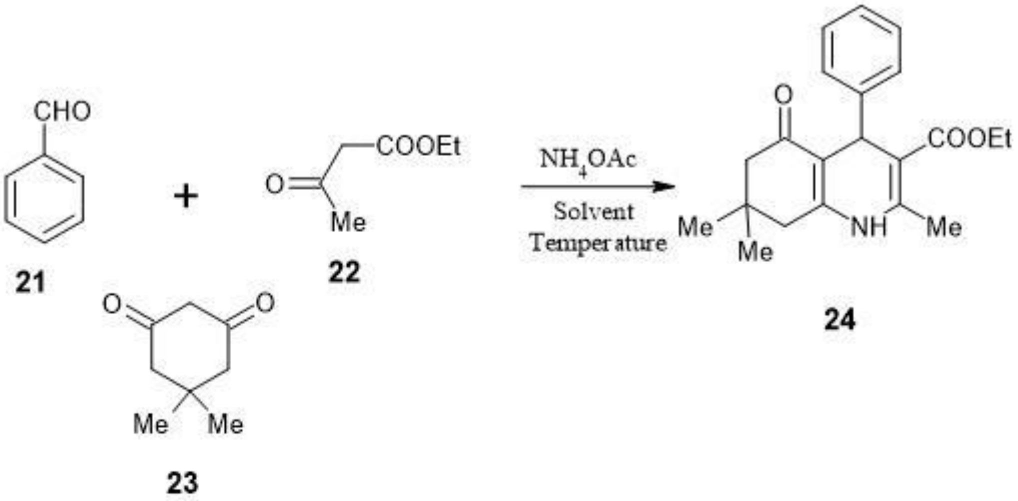
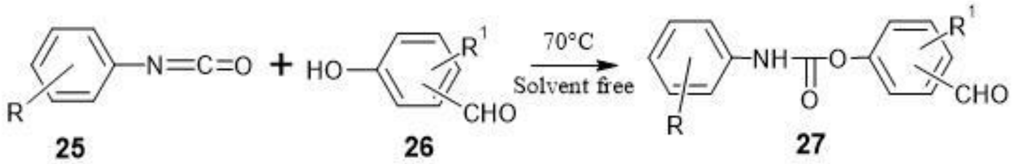
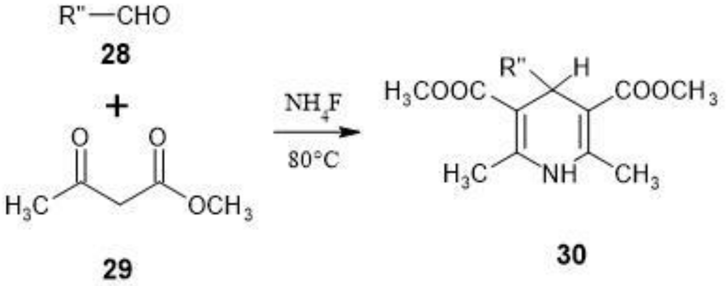


Fig.6 Synthesis of 1,4 DHP using eutectic solvents

4) Preparation of 1,4-Dihydropyridines bearing a Carbamate Moiety on the 4-Position: The preparation of various 1,4 DHPs having carbamate moiety on 4th position was done in two step reaction. Carbamate was prepared by reaction of different aldehydes with phenyl isocyanate. The resulting carbamate on reacting with methyl acetoacetate in the presence of ammonium fluoride gave 1,4 DHPs having carbamate moiety on 4th position. [23]

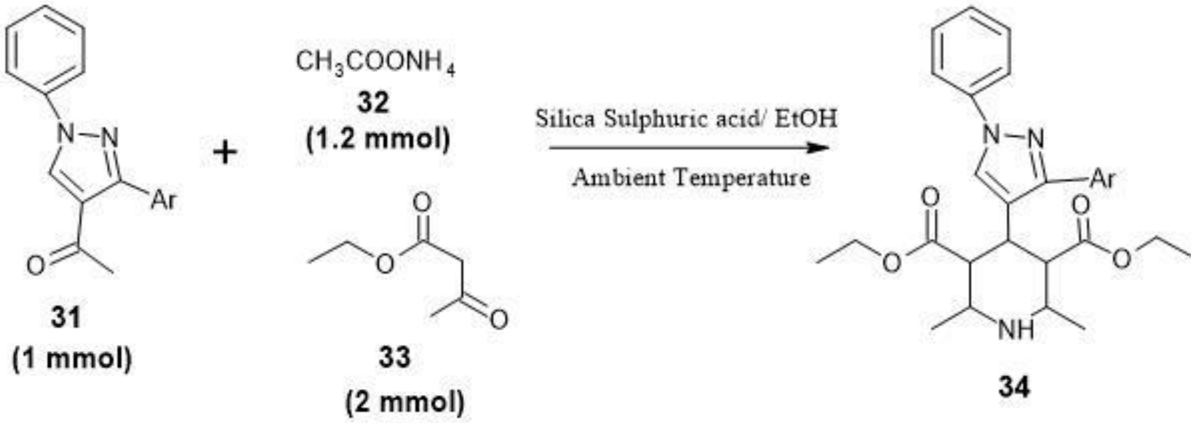


1. Synthesis of carbamate



2. Preparation of different 1,4- dihydropyridines from carbamates and methyl acetoacetate

5) Synthesis of novel bioactive 1, 4-dihydropyridine derivatives at ambient temperature and molecular modelling : A simple, mild , environmental friendly and efficient procedure using reusable silica sulfuric acid as a catalyst, at ambient temperature was given for the synthesis of biologically active 1, 4-dihydropyridines through solid-supported catalyst in a one-pot synthesis: 1 equivalent of substituted pyrazole carboxyaldehyde, 2 equivalents of ethyl acetoacetate, and 1.2 equivalents of ammonium acetate were stirred at room temperature, resulting in formation of corresponding 1,4-dihydropyridine. After optimising the reaction conditions for improvement in product yields, silica sulfuric acid was used in a catalytic amount of 0.25mmoles for 2.5 hours. A significant improvement was observed in the reaction time and product yield up to 96% [25]



Scheme 1. Synthesis of substituted 1,4- DHPs at ambient temperature

Table 1 : comparative summary of various green synthetic methods .

Sr. no.	Reactants	Reagent	Method	Time	Yield	conventional method	Reference
1	Alkyl aminocrotonate with an aldehyde and alkyl acetoacetate	Using sodium butyl mono glycol sulphate as aquesouos hydrotrope	Microwave	5 mins	35 to 97%	26 to 72% Yield	11
2	benzaldehyde: ethyl acetoacetate: ammonium bicarbonate		Microwave	25 mins	80%		15
3	Aryl aldehyde acetoacetic ester ammonium acetate	Tetra-methylguanidinium trifluoroacetate (TMGT) as ionic liquid	Ultrasound	1.4 to 2.3 h	84 to 90%	6 hrs time	19
4	Aldehyde, ethyl acetoacetate and ammonium acetate.	No catalyst	Ultrasound	25 to 70 mins	74% to 94%	-	20
5	Nitrobenz-aldehyde, methyl acetoacetate, ammonium acetate	in ionic liquid n-butyl pyridinium tetrafluoroborate	Heating 100° to 110° C	3 h	87% to 97%	36 to 70%	21
6	Substituted aldehyde, dimedone, ethyl acetoacetate and	in DES as solvent on heating	60° C	20 mins	95%	-	22

	ammonium acetate						
7	Carbamate, Methyl-acetoacetate and ammonium fluoride		80° C	17 to 24 mins	53 to 91 %	-	23
8	Aqueous Ethanol, substituted aldehyde, malononitrile dimethylacetylenedicarboxylate,2-fluoroaniline	Ultrasound		25 mins	89% to 96 %	-	24
9	Substituted pyrazole carboxy-aldehyde ethyl acetoacetate and ammonium acetate	Silica-sulfuric acid as catalyst	Ambient	2.5 h	96%	-	25

Conclusion

Hantzsch reaction has animportant role in synthesis of 1, 4- dihydropyridines which are considered to be one of the important class of pharmacologically active drugs. Various attempts have beenmade to make synthesis greener by changing the catalyst, solvents and procedures and to increase the yield, purity and activity of the products. Recent attempts are made by use of ionic liquids, Di eutectic solvents, Reusable catalyst like silica sulfuric acid , microwave and ultrasound waves for synthesis which have offered improvements such as fast reaction, simple operation, mild reaction conditions like room temperature, high yields and cost efficiency.

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Determination of Iron, Calcium, Potassium, and Sodium from Organic and Non-Organic Jaggery

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Abstract:
In India, the highest production of sugarcane was found in Uttar Pradesh and then second highest Maharashtra. In Maharashtra about 0.96 million hectares of area with production of 57.04 million tons with productivity of 74 tonns per hectare (2010- 2011). Chemical composition of jaggery consists of upto 50% sucrose, 20% invert sugars, moisture content 20% and the remainder made up of other insoluble matter such as ash, proteins and bagasse fines. It acts as important source of all important minerals and several vitamins.

Jaggery is easily available in the market and low-cost source of various minerals and vitamins. In the present study, we collected several jaggery samples mainly from Maharashtra, Uttar Pradesh and Gujrat including commercial jaggery as well as homemade jaggery. In different jaggery samples, determination of Iron content was carried by colorimetric method and the amount of calcium, potassium and sodium by flame emission spectrophotometry. It is was observed that, samples collected from Uttar Pradesh contains highest amount of iron, calcium, potassium and sodium.

Keywords: Jaggery, estimation of Fe, Ca, K, Na, Colorimetry, Flame Emission spectrophotometry.

Introduction:

Jaggery is a medicinal sugar and contains higher nutritional properties. Jaggery is very rich in iron and prevents anaemia. Jaggery supplements the requirement of calcium and iron in women and children. (Shinde et al. 2019; Singhet et al. 2016; Das et al. 2007) Jaggery is a natural traditional sweetener made by the concentration of sugarcane juice and is known all over the world. It is rich in important minerals like magnesium (70-90 mg), potassium (10-50 mg), phosphorus (20-90 mg), sodium (19- 30 mg), iron (10-13 mg), manganese (0.2-0.5 mg), zinc (0.2-0.3 mg), copper (0.1- 0.9mg), and chloride (5.3 mg) per 100 grams is present in this proportion. (Singh et al. 2015).

India is the largest consumer and the second largest producer of sugar in the world. Presently sugarcane is cultivated in an area of about 4.361 m hectares producing about 281.575 m tonnes of sugarcane annually. About 90% of production comes from Uttar Pradesh being the maximum producer. Total 32.5% of sugarcane produced is being utilized for producing jaggery. (Das et al. 2007) Sugarcane cultivation requires a tropical or subtropical climate with a minimum of 60 cm of annual moisture. Its cultivation is done on around 4 million hectares of land in India and its production has fluctuated between 230-300 million tons in past several years. (Kumbhar et al. 2015) Jaggery's colour varies from golden yellow to golden brown. Minerals present in jaggery strengthens human nervous system and helps to relax body muscles gives relief from fatigue and take care of blood vessels. The quality and price of jaggery is depending upon its external features like colour and texture. A best quality jaggery is judged by its features like golden yellow in colour, hard in texture, crystalline structure and its unique sweet taste, less in impurities like molasses and some crystals and low in moisture. The quality of jaggery is affected by many factors such as the variety of sugarcane grown, fertilizers used, quality of irrigation of water in particular soil region and method of clarification processing time, storage condition and packaging methods adopted. (Chitale et al. 2019) Sugarcane, member of grass family has potential to grow upto 4.5 m high under tropical condition. (Pradhan et al. 2007) There are mainly three forms of jaggery which are available in market viz., solid jaggery, liquid jaggery and granular jaggery.

Manufacturing of jaggery:

1) ***Liquid jaggery*** - It is obtained during making of jaggery. It is an intermediate of jaggery obtained in the form of semi-solid syrup during concentration of sugarcane. In 100 g of jaggery, the maximum carbohydrate, minerals and vitamins are sucrose 72-78 g, calcium 40-100 mg, magnesium 70-90 mg, phosphorus 20-90 mg, vitamin C - 7 mg, vitamin A - 3.8 mg, vitamin E -111.30 mg, vitamin D_2 -6.50 mg.

2) ***Granular Jaggery*** -It has similar process up to concentration of sugarcane juice. After this concentrated slurry is rubbed with wooden scrapper for formation of grains then it is cooled and sieved size should be less than 3 mm for better quality of granular Jaggery. pH is increased using lime up to 6.0-6.2 and temperature 120°C yielded quality granular Jaggery with high sucrose content of 88.6% and low moisture with good colour, friability and crystallinity.

3) ***Organic jaggery*** - Massive furnace is dug in ground then juice is poured in it and stirred continuously using bagasse as fuel. Then boiling sugarcane juice is cleaned using very small quantity of baking soda / juice of okra stem to bring up all the dirt and impurities. Then it is filtered with continuous stirring of about 2 h. the thickened juice is poured on another dry pan for next hour they turn over the thick liquid with large flat ladles, continued till liquid begins to take powdery consistency. A bit of natural lime and little organic coconut oil is added to it to get right consistency. It is given desired granular shapes. (Singh et al. 2016)

Materials and Chemicals:

All procured chemicals of analytical grade purity and distilled water were used. Colorimeter (Equiptronic EQ-651) and Flame Emission Spectrophotometer (Equiptronic EQ-

855A) instruments were used for the determination of Fe (II), Ca (II), K(I), Na (I) ions.

Methodology:

A. *Determination of Fe (II) ions by calorimetrically.*

Prepared 100 ppm Fe (II) solution by dissolving 0.176 g of ferrous ammonium sulphate and 5.0 mL of conc. H_2SO_4 in minimum quantity of distilled water and diluted to 250 mL with distilled water. For the preparation of 0.5 M Potassium hydrogen phthalate (KHP), dissolved 10.208 g KHP to 100 mL with distilled water. For 0.25% phenanthroline dissolved 0.25 g of 1, 10- phenanthroline to 100 mL with distilled water. (Amis et al. 1955) Calibration curve was prepared by taking 1.0, 2.0, 3.0. 4.0 and 5.0 mL of Fe (II) 100 ppm solution and 10 mL of KHP and 0.25% phenanthroline added to each flask respectively. Weighed 2 g of jaggery and dissolved in minimum quantity of distilled water and filtered the solution using filter paper. Collect the filtrate and add 10 mL of KHP and 0.25% phenanthroline added to each flask respectively.

B. **Determination of Ca^{2+}, K^+, Na^+ ions by using Flame Emission spectroscopy**
Determination of Ca (II) in jaggery sample:

Prepared 1000 ppm solution of Ca (II) by dissolving 0.692 g $CaCl_2$ to 250 mL with distilled water. Calibration curve was prepared by taking 2.0, 4.0, 6.0. 8.0 and 10.0 mL of Ca (II) 1000 ppm solution, dilute to 100 mL in standard measuring flask. Weighed 0.5 g of jaggery sample dissolved it to minimum quantity of distilled water and filter the solution with filter paper. Dilute the filtrate to 100 mL with distilled water.

Determination of K (I) in jaggery sample:

For the 1000 ppm solution of K^+, dissolved 0.477 g of KCl to 250 mL with distilled water. Calibration curve was prepared by taking 2.0, 4.0, 6.0. 8.0 and 10.0 mL of K(I) 1000 ppm solution, dilute to 100 mL in standard measuring flask. Weighed 0.5 g of jaggery samples and dissolved it to minimum quantity of distilled water and filter the solution using filter paper. Dilute the filtrate to 100 mL with distilled water.

Determination of Na (I) in jaggery sample:

Dissolved 0.635 g of NaCl and dilute the solution upto 250 mL with distilled water (1000 ppm of sodium ion solution). Calibration curve was prepared by taking 2.0, 4.0, 6.0. 8.0 and 10.0 mL of Na (I) 1000 ppm solution, dilute to 100 mL in standard measuring flask. Weighed 0.5 g of jaggery samples and dissolved it to minimum quantity of distilled water and filter the solution using filter paper. Dilute the filtrate to 100 mL with distilled water.

Result and discussion:

As estimated, the content of jaggery differs from place to place depending upon the type of soil and the way of preparation and manufacturing process. The homemade jiggery have dark colour and while commercial jaggery have light colour which indicates that the jaggery has undergoes several chemical processes such as refining process. Initially all the contents present in jaggery are derived from sugar-

Table 1: *Amount of Fe (II), Ca (II), K (I) and Na (I) in samples collected from different regions of India.*

Sr. No.	Jaggery Samples	Fe in mg/100g of Jaggery	Ca in mg/100 g of Jaggery	K in mg/100 g of Jaggery	Na in mg/ 100 g of Jaggery
1[a]	Gujrat	1.25	280	500	30
2[a]	Pune	1.25	360	200	40
3[a]	Ahmednagar	3.50	440	220	40
4[a]	Kolhapur	2.25	460	400	30
5[a]	Sangali	3.00	340	100	30
6[a]	Satara	1.25	160	400	10
7[b]	Banda	8.50	640	620	60
8[b]	U.P.	2.25	740	120	90
9[b]	Shahaganj	4.00	460	380	50

[a]samples: Commercial samples of jaggery, [b]samples: Homemade samples of jaggery, cane but the minerals like sodium is not the constituent of sugarcane and it is uptake from soil during cultivation period.

On the basis of colorimetric analysis Fe (II) maximum amount were observed in Banda sample and minimum amount in Pune, Satara and Gujrat samples. The highest amount of Ca (II) observed in Uttar Pradesh samples and lowest amount observed in Satara. The maximum amount of sodium was observed in Uttar Pradesh samples and minimum observed in samples collected from the Satara District. The amount of potassium was found to be maximum in Banda and minimum in Sangali. All elements are found moderate amounts in jaggery samples collected from Shahaganj and Ahamadnagar regions. (Table 1, entries 1-9)

Conclusion:

Jaggery is widely used in pharmaceutics and easily available in the markets. There are many forms of jaggery available in the market. We observed that, homemade jaggery is rich in all minerals as compared to commercial samples for the present study. The highest amount of calcium and sodium observed in Uttar Pradesh samples and lowest amount observed in Satara. The amount of potassium was found to be maximum in Banda and minimum in Sangali. Further investigation is in progress to correlate the effect of jaggery preparation procedure on composition of Jaggery.

Acknowledgment:

The authors are thankful to the Department of Chemistry, B. N. Bandodkar College of Science, (Autonomous) Thane and Vidya Prasarak Mandal, Thane for providing necessary facilities for research work.

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Photochromism in Spirooxazines

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Abstract:

Spirooxazines having high fatigue resistance are useful in different applications. This review emphasis on the use of photochromic properties of spirooxazine in the various fields as ion sensing probes, biomedical applications, biphotochromic, negative photochromism etc. The various substituent on the spiroxazine ring brings about changes in the photochemical responses and UV-Visible absorption. It opens up the opportunity in the research in the field of photochromism.

Key words:

Ion sensing probes, biphotochromic, molecular switches, negative photochromism, fluorescent quencher

Introduction:

Photochromic compounds are materials, changing their colour upon irradiation of certain wavelength, and reverting to the original colour upon irradiation of another wavelength or applying heat. Typical classes of photochromic compounds are spiropryans, spirooxazines, fulgides, and diarylethenes. The initial closed forms of spiropyrans and spirooxazines are colourless and undergo photoisomerization to the merocyanine forms by the cleavage of the C–O bond (Figure 1) Spirobenzopyran, spironaphthooxazine and naphthopyran undergo thermally reversible photochromic reactions. The first photochromic spirooxazine compounds synthesized belonged to the spiroindolinonaphthoxazine ring system. Generally, they were colourless in dilute organic solvents and polymer matrices and became blue upon exposure to UV light (Crano & Guglielmetti, 1999).

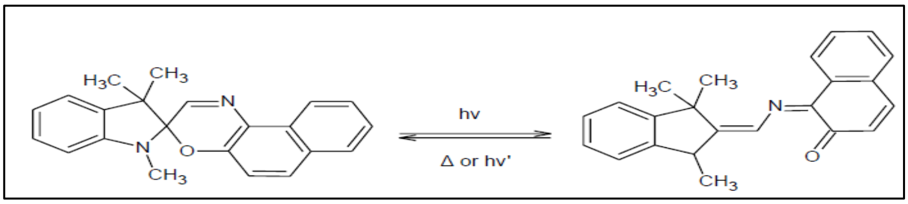


Figure 1 *Photoisomerisation of Spironaphthooxazine to merocyanine form*

Specific parameters such as absorption spectra and the molar absorption coefficients of the closed spiro- and open merocyanine forms, together with the photo coloration and photo bleaching quantum yields, rate constants and activation energies of thermal fading have been studied under continuous monochromatic irradiation (Kobatake & Irie, 2003).

Effects of Substituent on Photochromic properties

Substituent effects the photochromic properties based on the presence of it either on indoline or oxazine ring and also based on if it is an electron withdrawing or a donating group. A new spiro[indoline-naphthaline]oxazine derivative in figure 2a was synthesized and its photochromic properties in different solvents like trichloromethane and carbontetrachloride were studied. The piperidine group present act as electron-donating group in order to increase the electronic density of the molecular system having oxazino bridged system showing change in photochromic properties. Irradiation of this oxazine derivative with UV light of wavelength 365 nm showed absorption bands at 674 and 521 nm in trichloromethane and carbontetrachloride solution. Fatigue resistance studies showed that after 10-cycle irradiation of UV and visible lights, the absorbance was found to be 87.4% and 85.4% in trichloromethane and carbontetrachloride solvents respectively. The oxazine derivative also showed acidochromism properties in trifluoroacetic acid and triethylamine, showing colour change from colourless to blue indicating that the ring-opening was due to the formation of protonated photomerocyanine (PMCH) which was thermally stable and photo inactive. Studies showed that new spiro[indoline-naphthaline]oxazine derivative had high fatigue resistance hence making it applicable in sunglasses, optical switching, optical data storage etc.(H. Li et al., 2015). To design effective photoswitches it is necessary to study how the substituents affect the photochromic properties in spirooxazines. Comparative studies were done by synthesizing spirooxazines in figure 2b, having electron withdrawing and donating groups under similar conditions. The electron withdrawing group like nitro on both indoline and naphthoxazine ring improved the UV and visible light response. The trend was not found to be similar when methoxy group was present in the indoline ring. Influence of Gadolinium (III) binding on these spirooxazine having electron donating groups was altered on both the rings showed greatest photochemical responses. Many compounds did not show photoactivity because working condition were kept similar to biological system(Balmond et al., 2016). Spirooxazines were well suited for integration into Dye sensitised solar cell (DSSC) to fabricate photochromic solar cell due to their high fatigue resistance and stability as well as their strong absorption in the visible range. The naphthospirooxazines in figure 2c, with N-propanoic acid loaded on TiO_2 surface of solar cell was found to maintain its photochromic properties but its solar conversion efficiency was quite low (0.002%) compared to spiropyrans (Johnson et al., 2017). Spirooxazine containing sulfobutyl group in figure 2d, on the indoline ring was studied for its photochromic and kinetic properties of the metal complex formation. Formation of metal complex with merocyanine form of spirooxazine shows bathochromic shift of 8-20 nm. Metal complex formation and its stability depends on the metal ions(Fedorov et al., 2019). The novel spiro[indoline-quinoline]oxazine derivatives were synthesized having different substituents on indoline and quinoline rings. They were embedded into polymeric films and analysed by different techniques exhibiting excellent photochromic properties, high photostability and fatigue resistance (Zhou et al., 2020).

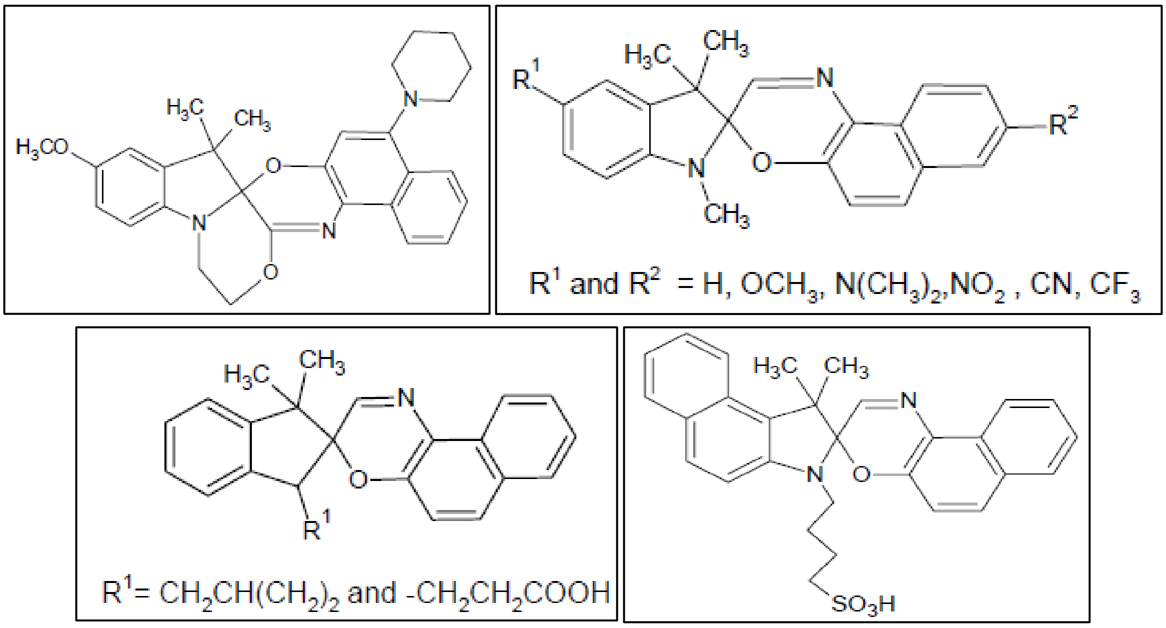


***Figure** 2 a, b, c and d*

Chelation of Spirooxazine: Ion sensing probes

Cation detection techniques are of extensive interest because of their widespread application in various fields, including biology, chemistry, clinical biochemistry, and environmental sciences. The Photochromic spriooxazines can also acts as highly sensitive and selective probe for optical detection of ions. The phtochromic spirooxazine derivative in figure 3a**,** prepared was evaluated for optical response towards heavy metal ions which selectively responded in the presence of Fe^{3+} ions. It produced nearly 100 nm shift in UV-visible spectrum and nearly 90-fold enhancement in fluorescence intensity in presence of one equivalent of Fe^{3+} ions. A shift in the absorbance band from 350 to 450 nm was observed when colourless spirooxazines solution in methanol: water (1:1) was treated with one equivalent Fe^{3+} ions to give yellow colour. It indicated the possible formation of complex of merocyanine form with Fe^{3+} ions. There was no change on addition of other heavy metal ions (Sahoo & Kumar, 2016). Study of Nonlinear optical spirooxazine compounds were done by team of researchers, they found that Spiroxazine transforms into metallic open merocyanine (MC) form giving rise to 10-21-fold higher static second order Nonlinear optical responses. Therefore, spirooxazine-to-merocyanine molecular switching can be used to distinguish alkaline earth metals and determine the efficiency of cation detection (Ye et al., 2017). Flourescent cyanide chemosensor based on photo switching poly(pyrene- 1-ylmethyl-methacrylate-random-methyl methacrylate-random- methacrylate spirooxazine) in figure 3b & c**,** (poly(PyrMMA-r-MMA-r-MSp)).

Pyrene was selected because of its use as a flouresecent probe in light responsive polymer. Photoisomerisation of this copolymer was studied both in solvent and solid-state film. On UV exposure, the copolymer showed blue colour and on exposure to visible light it turned colourless. The optical writing on the film were studied and found that even after 30 times repetitive erasing cycle, in presence of sunlight the polymer was not degraded. The solutions containing CN^- turned to yellow color after UV irradiation (365 nm) as a result of the complex formation with MC form of spirooxazine with CN^-, whereas the blank solution in the absence of CN^- remained colorless. This was in accordance with increases in intensity of the absorbance at 483 nm (Tran et al., 2019). Photochromic molecules can respond to external stimulations and undergo reversible conversion between different chemical structures, providing one photochromic molecule with multiple recognition states for targeting compounds. Quin et al., designed a facile sensor microchip with only one photochromic molecule (spirooxazine) to discriminate multiplex metal ions. The sensor chip performs in dark, ultraviolet, or visual stimulation, resulting in different molecular states of spirooxazine-metallic coordination and patterned fluorescent signals for analysis. By using this sensor microchip, 11 metal ions are discriminated. Furthermore, mineral water of 16 different brands and metal ions in human serum are distinguished (Qin et al., 2019). A novel spirooxazine (SPO figure 3d) derivative was designed for rapid detection of Hg2+ and CH3Hg+ in 1,4-dioxane. The chemical interaction of SPO and the selective cations proceeded through the ring opening after UV irradiation, followed by complexation reaction. The results indicated strong affinity of SPO for mercuric ions in presence of many other cations (Pattaweepaiboon et al., 2021).

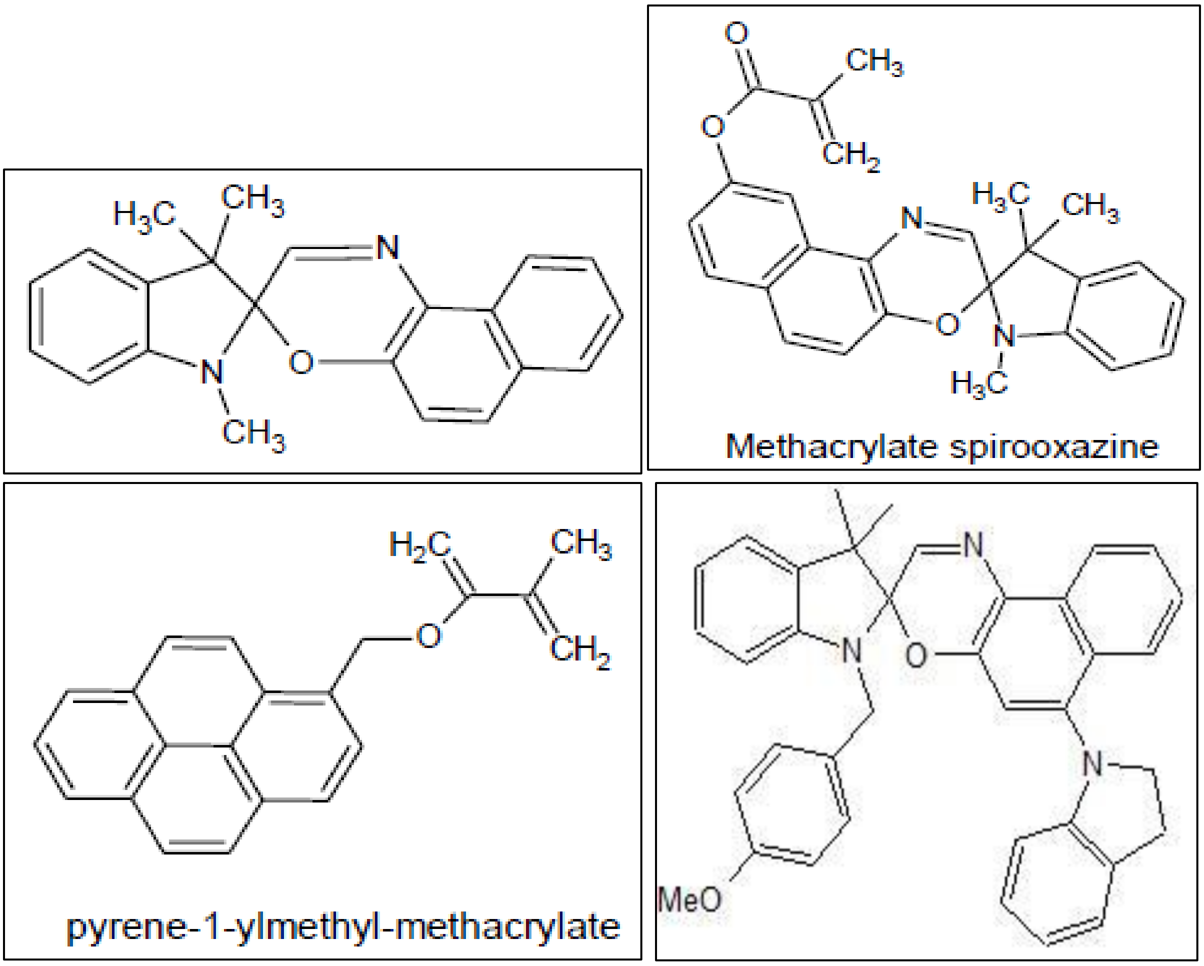


Figure 3: *a, b, c and d*

Spirooxazine dye on fibre

A photochromic spirooxazine dye in figure 4 is combined with a reactive dye to produce reversible colour change in cellulosic fibre. The novel dye synthesized was applied to cotton and photochromic colour change, fading speed were studied. When UV ray of 365 nm was irradiated on the spirooxazine derivative solution, the absorbance band was mainly observed in the range of 610-620 nm showing photochromism due to formation of open merocyanine form. The photochromic cotton fabrics was exposed to UV light ranging from 5 min to 22 h and found that fabrics showed colour change from reddish-orange to violet colour. Due to presence of permanent chromophore and reversible spirooxazine, the colour varies continuously with no constant pattern. The fading rate was found to be slower than photocolouration (Mokhtari et al., 2015). Modification of fibres with different materials to get functionalized textile is a future trend. A mixture of silica nanoparticle and photochromic spirooxazine dye was applied on cotton fabric to obtain multifunctional properties such as photochromic, hydrophobicity, antibacterial and ultraviolet (UV) blocking. Photochromic performance of the treated cotton was superior due to the silica nanoparticles with porous structure having free space for photochromic dye molecules to accomplish the photochromic reaction with excellent UV-blocking property due to the UV absorption ability of the spirooxazine and shows antibacterial activity due to presence of heterocyclic spirooxazine (Ayazi-Yazdi et al., 2017). The commercial development of photochromic textiles is limited mainly due to technical issues associated with application methods and performance. The use of supercritical CO_2 ($scCO_2$) dyeing method shows development of uniform colour and photochromic performance UV sensing smart textile using spirooxazine sea green dye (Abate et al., 2020).

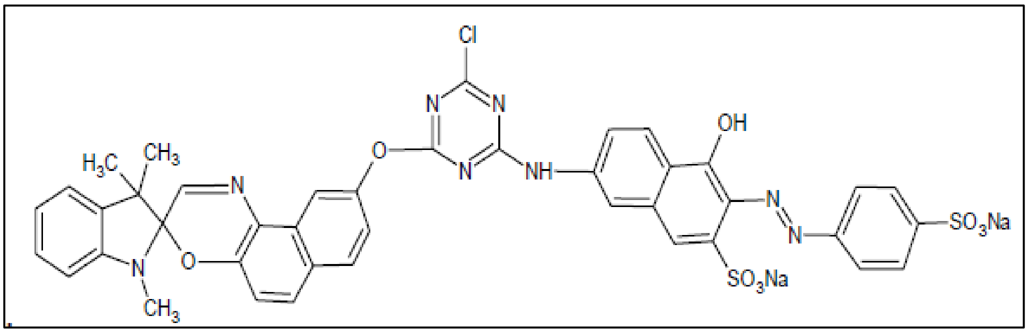
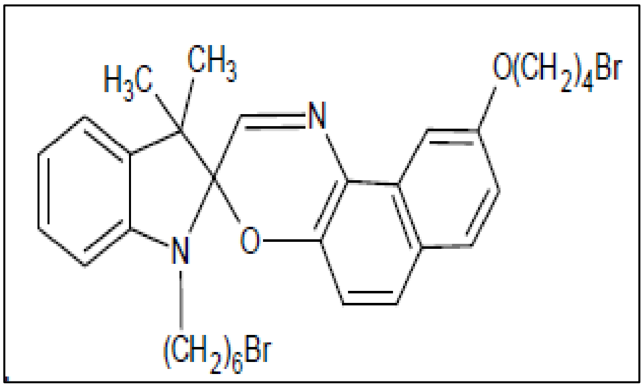
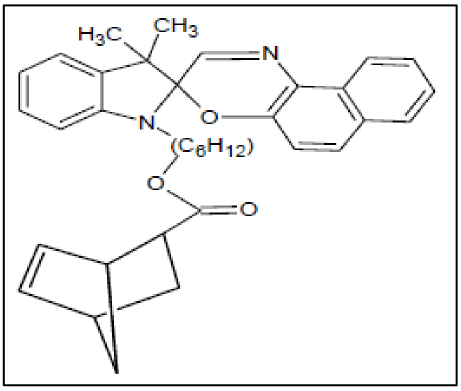


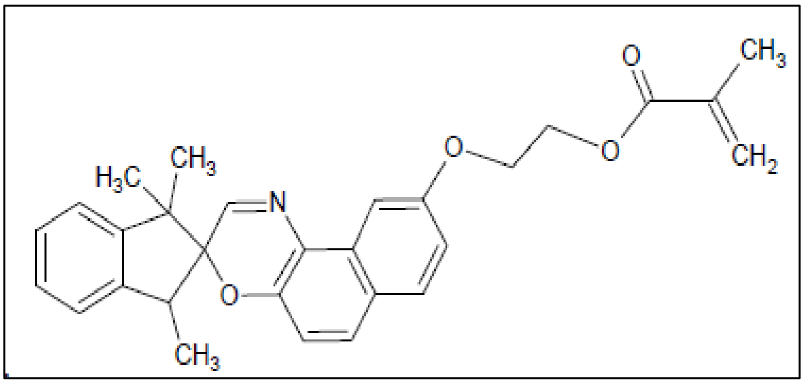
Figure 4

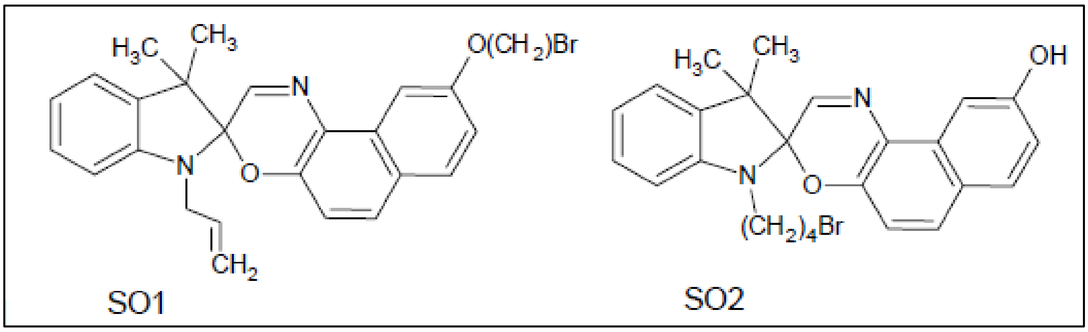
Spirooxazine linked Polymers

Spirooxazine (figure 5a) was grafted poly methyl methacrylate (PMMA), and study on the effects of hydrochloric acid on photochromic properties was carried out which showed good thermal stability of coloured photomerocyanine compared to spirooxazine ring form. PMMA is often preferred as polymer medium because of its moderate properties in transparency, stable performance, surface resistivity and weathering resistance (Wu et al., 2016). The functionalization of mesoporous silica material with photochromic units to mimic light gated ion channels using homopolymers of spirooxazines was successful. Spirooxazine norbornene (SPO-Nb) in figure 5b, monomers were synthesized first followed by ring opening metathesis polymerization of the monomer SPO-Nb performed in the presence of catalyst-modified mesoporous allyl silica films resulting in the formation of photochromic homopolymers PSPO in solution and covalently attached to the mesoporous films (Krohm et al., 2016). Photoswitchable fluorescent nanoparticles (PFNs) has been widely studied because of their potential biological application, such as ultrahigh-resolution imaging, two photon imaging. Photochromic fluorescent poly (MMA-co-SPO-co-TPE) nanoparticles with pendant spirooxazine (SPO) dye in figure 5c, and tetraphenylethylene (TPE) fluorophores attached to poly (methyl methacrylate) (MMA) backbone by semi-continuous polymerization was designed and its fluorescence quenching properties on exposure to UV and visible light was studied (X. Li et al., 2017). Spirooxazine (SO1 & SO2) in figure 5d & 5e, grafted and doped into PMMA through C-Br bonding sites, SO2 exhibited better photoresponse and slower bleaching in dichloromethane solution. SO1 and SO2 doped in PMMA exhibited better photoresponse property than those grafted in PMMA because spirooxazine was covalently attached with PMMA polymer backbone and encountered greater steric hindrance (Shi et al., 2017). Novel photochromic spirooxazine in figure 5f, were doped and grafted with water borne polyurethane (WPU) and their analysis showed that the light transmittance of modified WPU films decreased compared to pure WPU films but the water resistance and tensile strength were better. Also the thermal stability of spirooxazine in WPU film was enhanced(Cai et al., 2019).









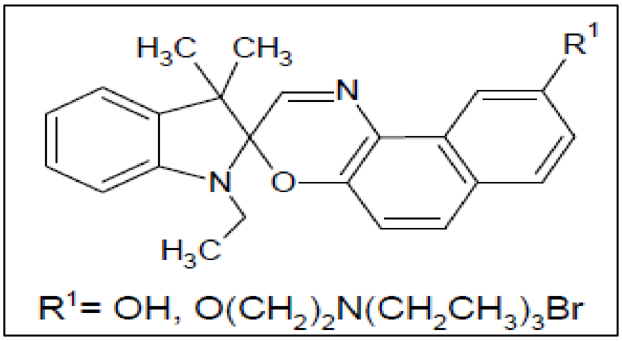
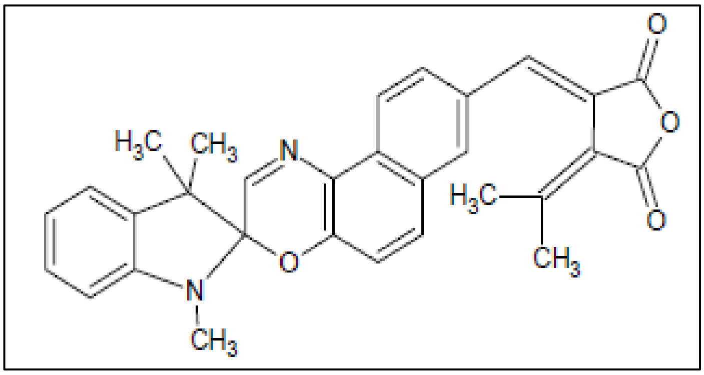


Figure 5: *a, b, c, d, e, f*

Biphotochromic system

Combining two photochromic molecules will give rise to biphotochromic molecules which can enhance the properties and open up many applications in the field of molecular switches and memory devices. Spirooxazine and fulgides system were combined by naphthalene ring figure 6a**,** and switching behaviour, theoretical study of optical /spectroscopic properties and electronic structures were carried out by density functional theory to show the working of biphotochromic system as four states Nonlinear optical (NLO) switches. Compared to spirooxazine series the photomerocyanine series in biphotochromic system showed more extensively conjugated moieties which may promisingly have large hyperpolarizabilities to be devised as NLO systems(Yuan et al., 2016). Boronic acid derived salicylidenehydrazone (BASHY) dyes was sandwiched between photochromic spirooxazine and fulgides system shown in figure 6b. It showed the properties of molecular switch with multiple responses of optical absorption, florescence emission and quadratic NLO which can be applied for florescent imaging in biological context or information processing (Yuan et al., 2019).



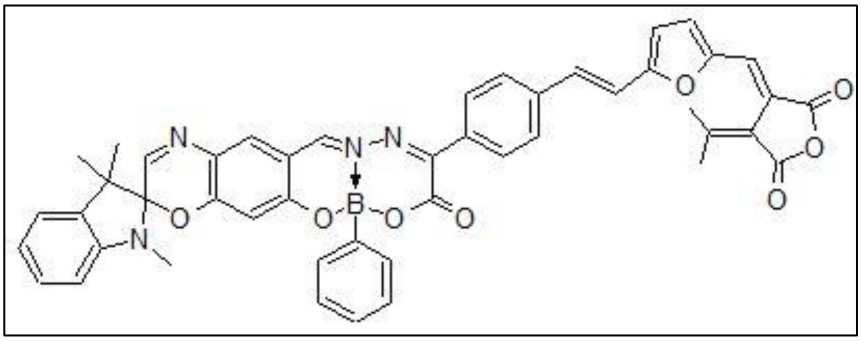


Figure 6: *a and b*

Biological application

Sensor chips composed of photochromic spirooxazine-metallic complexes are used to detect natural amino acids by distinct fluorescent pattern for each amino acid. Metal ions combined spirooxazine provides abundant sensing information under distinct conditions as dark, UV and visible light irradiation for the identification of mixtures of amino acids which can be extended to perform on human serum (Qin et al., 2015). Spironaphthoxazine derivative in figure 7, photochromic switch as a potential photochromic FRET- quencher for RESOLFT microscopy was synthesized and demonstrated that spirooxazines can be used in living cells, it is possible to use them to modulate the fluorescence of a covalently attached fluorescent dye in biological media (Xiong et al., 2018).

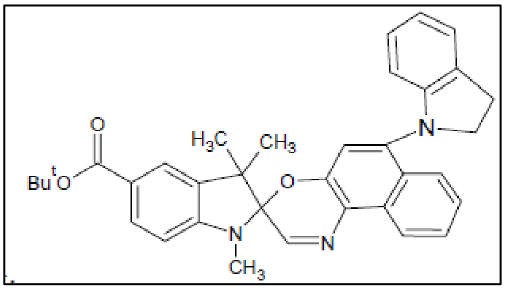


Figure 7

Negative Photochromism

An unusual class of spirooxazines that exhibits negative photochromism has been developed, the azahomoadamantyl-spirooxazines in figure 8a**,** in which the ground state is the photomerocyanine (PMC) form. Integration of phenanthroline into the spirooxazine backbone generates photochromic ligands that when bound to paramagnetic metal centers exhibit high photoresponsivities. The study suggests that the optical gating occurs at the single- molecule level in the solid state, this opens up possibilities for single-molecule opto-spintronic devices as well as a broad array of applications requiring optically gated spin/charge states (Paquette et al., 2018). Visible-light-responsive conjugated polymer nanoparticles (CPNs) doped with a reverse photochromic spirooxazine dye in figure 8b, has been developed that has a thermally stable merocyanine form. Off-to-on fluorescence switching occurs when the merocyanine is switched to its non-quenching spirooxazine form. The on-state fluorescence intensity is more than 100 times greater when photoswitching occurs via fluorescence resonance energy transfer (FRET) from the CPNs. Photokinetic measurements and simulations explaining how FRET excitation of MC dye yields higher fluorescence has been studied in this research (Zhang et al., 2018).

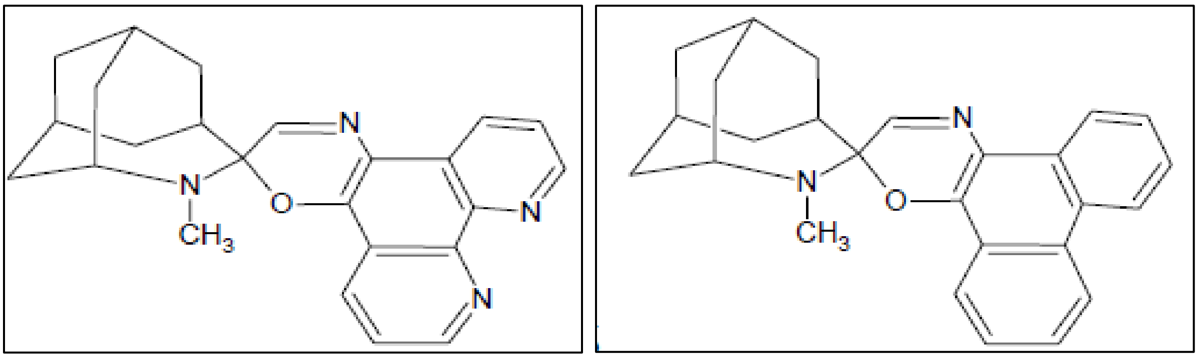


Figure 8: *a and b*

Triplet state photosensitised photochromisim

Series of azo-, stilbene and spirooxazine (SOPY and SOBPY in figure 9)**,** molecules were designed containing pyridine ligand which were coordinated with tricarbonylrhenium(I) diimine complex to study their triplet state photosensitised photochromisim. The photosensitization of the photochromic ring-opening reaction could be achieved with the metal ligand charge transfer (MLCT) excited state of the Rhenium (I) complexes. The photo-chromism could be extended from the UV region in the pure organic system to the lower-energy visible light region in their coordination compounds hence giving rise to near infrared (NIR) responsive photochromism systems (Ko & Yam, 2018).

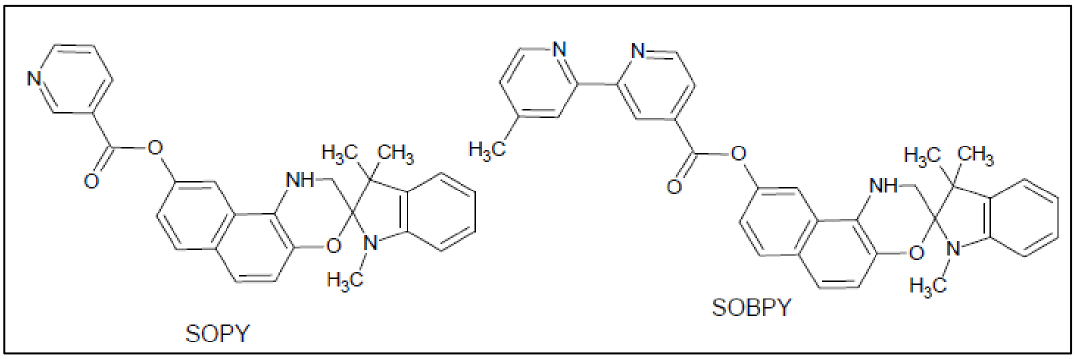


Figure 9

Conclusion

In summary, spirooxazine has shown many applications due to its photchromic properties. Due to its high fatigue resistance, thermal stability, complex formation with different metal ions, high photostability, reverse photochromism, biphotochromic molecule formation, grafting with PMMA and linkage with textiles fibres gave rise to commercial application in the field of biological sensors, molecular switches, chemosensors, photochromic FRET-quencher for RESOLFT microscopy and NLO switches. There is a scope for improving these properties for more applications in the photochromic based functional devices.

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Allium Cepa Dye and Its Application

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Abstract

The efficiency of dyeing cotton fabric with natural dye obtained from kitchen waste of dry skin extract of *allium cepa*. The scaly skin of onion produces orange- brown natural dye which can used for dyeing textiles. In the present study, dyeing with onion dry/papery skin has been shown a great dyeing results. *Allium cepa* dye eliminates the use mordents or fixatives during process due to rich in tannin. The study advancing the dyestuff chemistry.

Keywords –

Onion, pelargonidin, cotton fabric, shibori technique.

Introduction-

Natural dyes added colour to the substances. Such substances with considerable colouring capacity are widely employed in the production of consumer products, including paints, textile, food, cosmetics and many more. Majority of it, is isolated from plant origin and moderated with metallic salts (Chris Mclaughlin 2020). M G Silva *et*, *al* (2018) suggested that onion skin extract acts as antimicrobial, anti-inflammatory and anti UV properties on fabric. Since, onion is rich in polyphenol and responsible for colouration. The same properties were also ascribed by Lucia Pucciarini 2019 for the golden colour of onion papery skin. In 2020, Mohamed z. M showed that pancreatic enzymes are for textile dyeing. Onion contains various phytochemicals including alkaloid- quercetin, flavonoids, anthocyanidins, tannins, salicylic acid and provide an excellent source of vitamin A, C, E and antioxidants. Many researchers used high end instruments for the extraction of dyes from various natural resources. But due to pandemic situation, college laboratory is not accessible, to utilised time in positive way, homemade dyes were synthesised and applied for the dyeing fabric.

Methodology-

Material- dry skin of onion, burner, hot bath, cotton fabric, vinegar

Method-

Source: after using onion for culinarians the waste pepery skin of onion was used for the extraction of dyes.

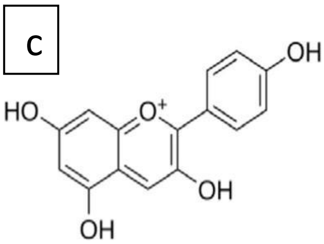
Extraction of dyes

Dried onion (10gm) place stainless stain bowl and added 100 ml of water, boiled and observe the change in colour of water. The coloured water was reduced to get concentrated dyes. The onion skin was removed with spatula from bowl and added vinegar: water, (4:1) in it. The pre-wet fabric is immersed into the dye bath and heated it for 30-60 min. The dye bath was stirred, using a spoon to remove stuck material to the stainless-steel bowl, to submerge the fabric and free from bubbles to achieve even colour.

After the fabric set in dye bath and absorption of colour by fabric, unattached dye was removed by washing with chilled water. Dried the fabric.

Structure of onion dye

The dye stuff present in onion skin is called pelargonidin (5, 5, 7, 4-tetrahydroxyantocyanidol. The amount of colouring pigment present varies from 2.0 to 2.25%.

		
a. *Allium cepa*	***b***. *Dried skin*	**c.** Molecular structure of pelargonium

Results and discussion:

The waste dried skin of red onion was selected for dyeing the cotton fibre bye shibori technique. The main purpose of extraction is to transfer colouring component present in source to solvent medium for producing different shades of bright colours. The diluted dye was in orange-reddish in colour while after concentration it give dark brownish in colour. The fabric dyes with it as follows-

before

after

Conclusion

The dye is eco-friendly, useful and employing the waste material for its usefulness.

Acknowledgement

Authors is very much thankful to, V. P. M.'s B.N. Bandodkar college of science, Thane.

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Estimation of Fluoride Ions from Different Water Samples of Nearby Water Bodies Using Colorimeter

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Abstract

In the context of human health, fluoride is mainly utilized to improve dental health and skeletal health. As the concentration of fluoride ions present in water samples is considerably important, we have collected wide range of water samples from thane district to Konkan district out of various sources like hand pump, lake, well and tap water. Initially Quantitative analysis was carried out for fluoride ions present in the standard sodium fluoride solution by calibration curve method. Various concentrations of sodium fluoride solutions were treated with Zirconyl nitrate and alizarin red reagent which formed yellow-orange complexes. λ_{max} for highest concentration of sodium fluoride solution from considered calibration curve range is 530nm. Collected water samples were also estimated for its fluoride content colorimetrically. The unknown concentrations of fluoride ions in ppm from collected water samples were estimated by extrapolating the calibration curve plot.

Keywords: Colorimeter, Absorbance, Calibration curve, Absorption, Alizarin Red-S, Zirconyl nitrate, Fluorizirconate.

Introduction: -

According to the World Health Organization recommendation limit of fluoride in drinking water is 1.5 ppm, which is also the upper limit for fluoride in drinking water for several other countries such as Canada, China, India, Australia, etc. Fluoride has presence in all natural water. Seawater contains 1.2-1.5 ppm of fluoride. Freshwater concentrations are usually lower ranging from 0.01 to 0.3 ppm (1). Fluoride deficiency can lead to tooth decay and possibly osteoporosis. Consuming enough fluoride can make tooth decay less likely and may strengthen bones. The addition of fluoride (fluoridation) to drinking water that is low in fluoride or the use of fluoride supplements significantly reduces the risk of tooth decay(2).

There are various methods to estimate the fluoride contain in water:

1) Coagulation and precipitation
2) Membrane process which include a) reverse osmoses {RO} b) Dialysis c) electro dialysis
3) Ion exchange process
4) Electro-coagulation (EC) process
5) Adsorption

One way to avoid the fluoride from tap water is to purchase a water filter. Spring Water is another way to avoid fluoride from tap water. Most brands of spring water contain very low levels of fluoride. Water Distillation is a third way to avoid fluoride. Water distillation will remove most of the fluoride (3).

Research methodology-

Material: - 100 cm^3, 250 cm^3 standard measuring flask, beaker (100 cm^3, 250 cm^3, 500 cm^3), pipette (25 cm^3, 10 cm^3), graduated pipette (2 cm^3, 5 cm^3, 10 cm^3), test tubes, weighing balance, wire gauze, glass rod.

Chemical: -

Reagent A: - Dissolve 0.188 g of Alizarin red –S in 250 cm^3 of distilled water (store in dark cool place)

Reagent B: - Dissolved 0.073g of $ZrO(NO_3)_2.2H_2O$ in about 150 cm^3 of distilled water. Added 8.3 cm^3 of concentrated H_2SO_4 and diluted it up to 250 cm^3.

Methods: -

Colorimeter follows the principle of Beer-Lambert's Law. The Beer-Lambert law states that there is a linear relationship between the concentration and the absorbance of the solution, which enables the concentration of a solution to be calculated by measuring its absorbance. A typical human eye will respond to wavelengths from about 380 to 750 nanometres. The experiment is carried out at wavelength of 530nm on colorimeter for estimation process. When a Zirconyl nitrate salt is added to a solution of hydroxy anthraquinone (Alizarin) in acid solution, wine red coloured complex is formed. This when comes in contact with fluoride ion present in solution, gets bleached due to the formation of colourless Fluorizirconate $(ZeF_6)^{-2}$ anion. The alizarin reaction results in a series of colour from wine red to yellow- orange. As the concentration of fluoride ion present in solution increases, the intensity of colour decreases thus absorbance's also decreases. Here, the concentration of fluoride ions is inversely proportional to absorbance.

Calibration Curve and estimation of collected samples:

1) 10 cm^3 of 100 ppm solution of sodium fluoride is diluted up to 100 cm^3 with distilled water to prepare 10 ppm sodium fluoride solution which was used for further dilutions.

2) Ten different standard solutions were prepared by addition of 2cm^3, 4cm^3, 6cm^3, 8cm^3, 10 cm^3, 12cm^3, 14 cm^3, 16cm^3, 18cm^3 and 20cm^3 of 10 ppm solution of sodium fluoride into ten labelled 100 cm^3 standard measuring flasks respectively of 0.2 ppm, 0.4 ppm, 0.6 ppm, 0.8 ppm, 1.0 ppm, 1.2 ppm, 1.4 ppm, 1.6 ppm, 1.8 ppm, 2.0 ppm as shown in **Table 1**. As well as 10 cm3 of all collected samples were taken in another four different standard measuring flasks containing sample A, sample B, sample C, sample D.

3) Then 5 cm^3 of reagent A was added to each flask. Then added 25cm^3 of distilled water to each flask. Shaked it well. After an interval of 10 minutes 5cm^3 of reagent B was added to each

flask and diluted with distilled water upto the mark and kept aside for 30 minutes in dark place. For these solutions the absorbance was measured at 530 nm and a calibration curve was plotted for concentration of fluoride ion versus absorbance measured.

Picture (a): 100 cm^3 standard measuring flasks containing different ppm concentration of fluorides ions solution for calibration curve.

Picture (b): 100 cm^3 standard measuring flasks of various water sample containing unknown amount of fluorides ions

Observation table:

Sr. No.	**Concentration of fluoride ion in ppm**	**Absorbance**
1	0.2	0.19
2	0.4	0.18
3	0.6	0.17
4	0.8	0.16
5	1.0	0.15
6	1.2	0.14
7	1.4	0.13
8	1.6	0.12
9	1.8	0.11
10	2.0	0.10
11	Sample A	0.15
12	Sample B	0.12
13	Sample C	0.17
14	Sample D	0.18

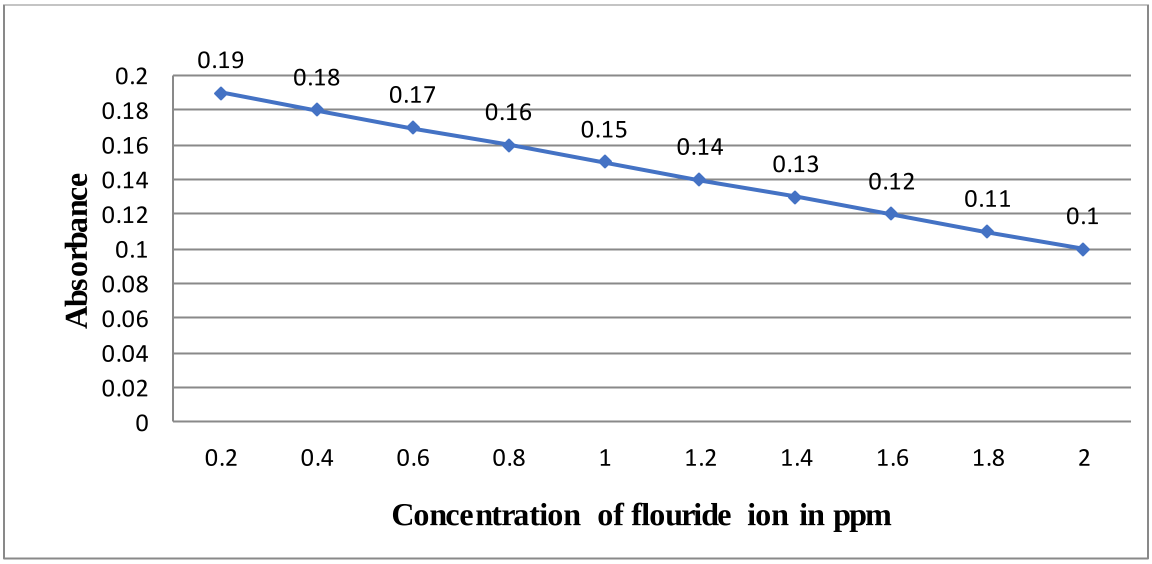
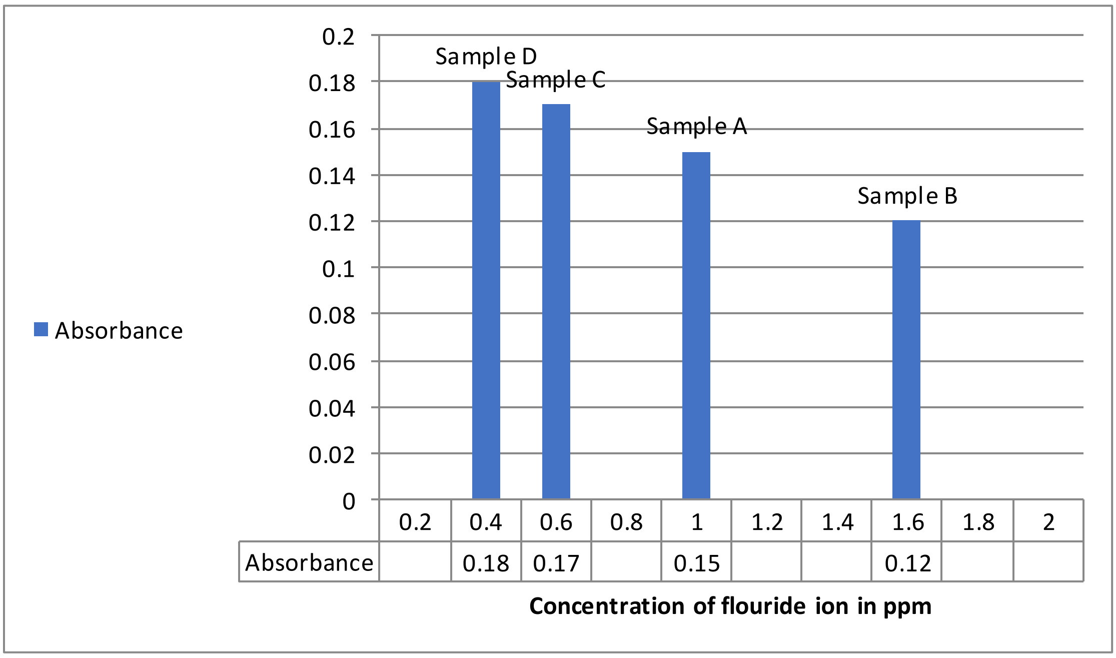


Figure 1. Calibration curve plot for concentration of fluoride ions in ppm against absorbance

Sample A: - Talav Pali water, Thane
Sample B: - Konkan region water
Sample C: - Hand pump water, Thane
Sample D: - Tap water of B. N. Bandodkar College, Thane



	0.2	0.4	0.6	0.8	1	1.2	1.4	1.6	1.8	2
Absorbance		0.18	0.17		0.15			0.12		

Figure 2. Calibration curve plot for concentration of fluoride ions in ppm against absorbance for sample A, sample B, Sample C and Sample D.

Result: -

The obtained value of absorbance of sample A is 0.15, sample C is 0.17 and of sample D is 0.18 which belongs to 0.7ppm, 0.5ppm, 0.4ppm concentration of fluoride ion in the sample respectively. Sample B has shown absorbance of 0.12 which belongs to concentration 1.6 ppm.

Conclusion: -

Fluoride ion concentrations from Sample A, Sample C, Sample D are coming under tolerance limit which indicates that they are edible. For Sample B, fluoride ion concentration is slightly higher than that of the tolerance limit which is acceptable as this sample was collected from the river which was completely contaminated after the flood.

Acknowledgement: -

Author is very much thankful to, V. P. M.'s B.N. Bandodkar College of science, Thane and Department of chemistry for providing necessary equipment for carrying out the experiment.

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Effective Adsorption of Fluoride on Low Cost Bioadsorbent Mixture of Charcoal with *Malus Domestica Peel* and *Cocos Nucifera* Husk.

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Abstract:

Fluoride is found to be one of the anionic contaminants, which are found in excess on the surface or ground water that leads to hazardous effect on the living organisms. In present work, only dried apple peel powder, only coconut husk powder, dried apple peel powder with charcoal and coconut husk powder with charcoal is been investigated with fluoride rich water. The study includes treatment of adsorbents on fluoride ion present in the solution, factors affecting adsorption and adsorption capacity of adsorbent with varying quantity. After adsorption, resultant fluoride ion content was estimated by well-established calibration curve method using spectrophotometer as an instrument.

Keywords:

Adsorption, fruit peel waste, bio adsorbent, activated carbon.

Introduction:

The presence of naturally occurring fluoride ions in drinking water allows its easy entrance in the body via gastrointestinal tract. Heightened fluoride >1.5mg/L concentration can induce birth, reproduction as well as immunological defects, dental and skeletal fluorosis [1]. Numbers of methods are available for removal of fluoride ions from aqueous solution which includes chemical precipitation, ion exchange, biological degradation, solvent extraction and adsorption. Among all these methods adsorption is most popular, simple and effective technique. This process can minimize or remove fluoride ion and thus have wide range of applications in waste water treatment. Conventional adsorbents and non-conventional adsorbents are two types of adsorbents. Activated charcoal is the form of carbon which is processed to have low volume pores that increases the surface area available for adsorption. Activated carbon is an example of conventional adsorbent which is commonly used for removal of various pollutants from waste water. Non-conventional adsorbents such as fruit peel waste, agricultural waste, plant waste, living and non-living mass which also referred as bio adsorbents. Our country is the second largest producer and consumer of fruits which also indicates the generation of million tons of fruit peel waste, which can be effectively used for removal of fluoride ions. Advantages of abundantly available, Low cost fruit peels are it has good adsorption capacity and less disposal problem after absorption [2].

Adsorption capacity of fruit peels waste and factors affecting it:

Adsorption is described as a process by which solids holds molecules of gases/ liquids on its thin films. Adsorption processes are of two types: physical and chemical adsorption [3].The type of adsorption used in above research project is physical adsorption. Adsorption capacity of fruit peel depends on size, surface area and relative affinity towards adsorbate [4]. The relative affinity of adsorbent depends on: - 1) Thickness 2) density of adsorbent 3) radius of fibres 4) temperature. NaF is used as an adsorbate as it reflects the properties of solution containing fluoride.

Material and Methods:

Materials:

Standard measuring flask (100 cm^3, 250 cm^3), beaker (100 cm^3, 250 cm^3, 500 cm^3), pipette (25 cm^3, 10 cm^3), graduated pipette (2 cm^3, 5 cm^3, 10 cm^3), test tubes, weighing balance, wire gauze, glass rod, charcoal powder, coconut husk powder, oven, funnel, filter papers, dried apple peels powder, colorimeter.

Chemicals:

Sodium fluoride salt, Alizarin red-S, Zirconyl nitrate, Distilled water.

Methods:

The Colorimeter worked on the principle of the Beer-Lambert’s law and operated in the visible range of the spectrum. The colorimetric reagent formed during the analysis was Zirconyl Alizarin complex, for which the λ_{max} value obtained was 530 nm. The Zirconyl Alizarin complex has a deep reddish brown color. This when came in contact with fluoride ions, bleaches due to the formation of colorless fluorizirconate anions. As the concentration of fluoride increases, colorless fluorizirconate anion increases in concentration which decreases the intensity of absorbance. The Colorimetric analysis was used for its simplicity, convenience and availability in the institute.

1) **Stock solution of sodium fluoride (100 ppm):** Dissolved 0.055 g of sodium fluoride into 250 cm^3 of distilled water in a standard measuring flask.
2) **Reagent a**: dissolved 0.188 g of alizarin red-s into 250 cm^3 of distilled water.
3) **Reagent b**: Dissolved 0.073g of $ZrO(NO_3)_2.2H_2O$ in about 150 cm^3 of distilled water. Added 8.3 cm^3 of concentrated H_2SO_4 and diluted it upto 250 cm^3.

Calibration curve method:

1) 10 cm^3 of 100 ppm solution of sodium fluoride is diluted up to 100 cm^3 with distilled water to prepare 10 ppm sodium fluoride solution which was used for further dilutions.
2) Ten different standard solutions were prepared by addition of 2cm^3, 4cm^3, 6cm^3, 8cm^3, 10 cm^3, 12cm^3, 14 cm^3, 16cm^3, 18cm^3 and 20cm^3 of 10 ppm solution of sodium fluoride into ten labeled 100 cm^3 standard measuring flasks respectively of 0.2 ppm, 0.4 ppm, 0.6 ppm, 0.8 ppm, 1.0 ppm, 1.2 ppm, 1.4 ppm, 1.6 ppm, 1.8 ppm, 2.0 ppm as shown in **Table 1**.

3) Then 5 cm^3 of reagent A was added to each flask. Then added 25cm^3 of distilled water to each flask. Shaked it well. After an interval of 10 minutes 5cm^3 of reagent B was added to each flask and diluted with distilled water up to the mark and kept aside for 30 minutes in dark place. For these solutions the absorbance was measured at 530 nm and a calibration curve was plotted for concentration of fluoride ion versus absorbance measured.

Sample preparation and treatment on fluoride solution:

The adsorbent apple peels, coconut husk and charcoal were finely chopped and then apple peels and coconut husk dried in oven at around 109º C (air dry) for around 2 to 4 hours. The different amount and different mixture of adsorbents were added to 2.00 ppm standard solution of NaF, as shown table no.2. The mixture was shacked vigorously and these samples were then allowed to stand overnight. These samples then filtered to get cleared solution. Then 5 cm^3 of reagent A was added to each flask. Then 25cm^3 of distilled water was added to each flask. Shaked it well. After an interval of 10 minutes 5cm^3 of reagent B was added to each flask and diluted with distilled water upto the mark and kept aside for 30 minutes in dark place. For these solutions the absorbance were measured at 530 nm and a calibration curve was plotted for concentration of fluoride ion versus absorbance measured.

Picture (a): dried samples of Charcoal powder, apple peel powder, coconut husk powder

Picture (b): 100 cm^3 standard measuring flasks with adsorbent and fluoride solution before dilution

Picture (c): 100 cm^3 standard measuring flasks after dilution of fluorides solution (filtered from soaked adsorbent)

Picture (d): Colorimeter while performing the experiment

Observation table:

Flask no.	Type of adsorbent	Wt. of adsorbent in grams.	Vol. of NaF in 10ppm	Conc. of F^- ions (ppm)	Conc. of F^- ions (mg/100cm^3)	Absorbance
1.	Apple peels powder	0.025	20	2.0	0.2	0.10
2.	Apple peels powder	0.05	20	2.0	0.2	0.09
3.	Apple peels powder	0.075	20	2.0	0.2	0.07
4.	Apple peels powder	0.1	20	2.0	0.2	0.08
5.	Charcoal powder	0.025	20	2.0	0.2	0.14
6.	Charcoal powder	0.05	20	2.0	0.2	0.17
7.	Charcoal powder	0.075	20	2.0	0.2	0.16
8.	Charcoal powder	0.1	20	2.0	0.2	0.15

9.	Charcoal powder + coconut husk powder	0.025	20	2.0	0.2	0.15
10.	Charcoal powder + coconut husk powder	0.05	20	2.0	0.2	0.17
11.	Charcoal powder + coconut husk powder	0.075	20	2.0	0.2	0.18
12.	Charcoal powder + coconut husk powder	0.1	20	2.0	0.2	0.18
13.	Charcoal powder + apple peels powder	0.025	20	2.0	0.2	0.18
14.	Charcoal powder + apple peels powder	0.05	20	2.0	0.2	**0.21**
15.	Charcoal powder + apple peels powder	0.075	20	2.0	0.2	**0.23**
16.	Charcoal powder + apple peels powder	0.1	20	2.0	0.2	**0.21**

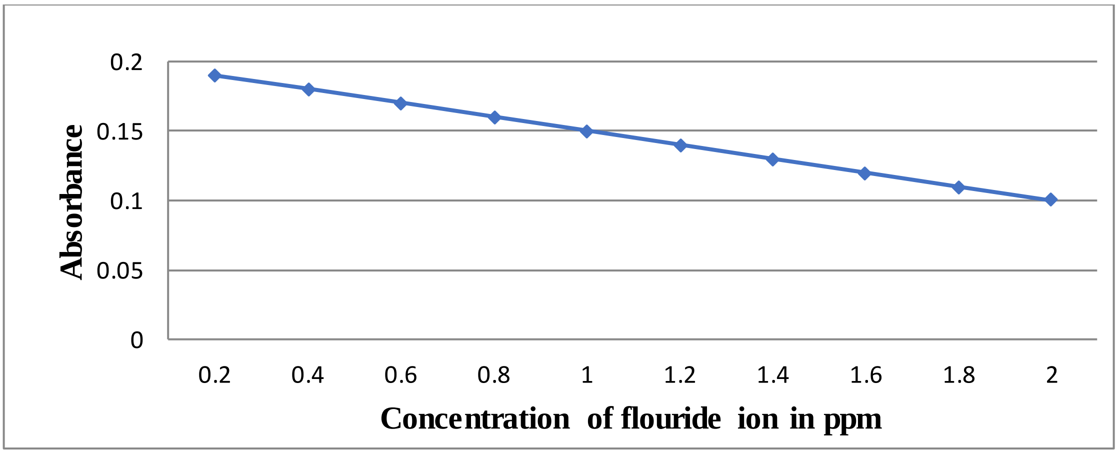

Figure 1. Calibration curve plot for concentration of fluoride ions in ppm against absorbance.

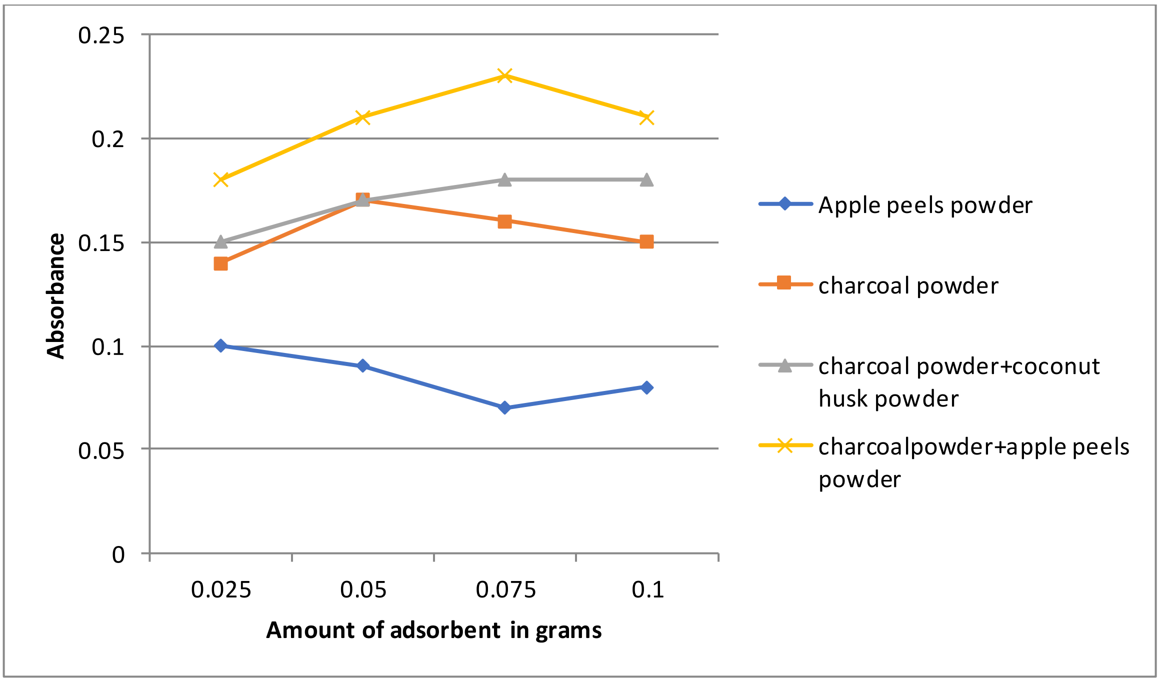

Figure 2. Relative plot for different amounts of adsorbent in grams for various mixtures of adsorbents against absorbance.

Results and Discussion:

The above method was based on absorbance property at specific wavelength of light for the colored complexes. The absorbance of the sample was determined by colorimeter and concentration of fluoride ion after adsorption with different adsorbents was found out by using calibration curve method. Only apple powder as well as only charcoal has also shown noticeable adsorption. The results have shown that charcoal powder with coconut husk powder and charcoal powder with apple peels powder is effective for adsorption of fluoride ions on its surface. About 2.0 ppm of fluoride is reduced to less than 0.2 ppm fluoride.

Conclusion:

Activated carbon/charcoal is a good adsorbent in extraction of fluoride ion. Addition of apple peels powder and coconut husk powder increases the adsorptivity of charcoal towards fluoride ion. This provides an alternate method for adsorption of fluoride ion in cheap and effective manner. The study can be continuing by extracting fluoride ion from waste water, helps in waste water management.

Acknowledgement:

Authors are thankful to Chemistry Department of V.P.M.'s B. N. Bandodkar College of Science, Thane, for providing laboratory facilities, required chemicals and instruments.

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Bioremediation Solution to Remove Pollution

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Abstract:

Bioremediation is a process that utilizes the living organisms, mostly microbes and plants, to degrade and reduce or detoxify waste products and pollutants. But recycling can also be the way of bioremediation. we have not only polluted our planet but also the space and other planets above us. Many artificial satellites , robotic machines are still in space, left on grounds of others planets as E-waste,. Very few organizations are working towards bioremediation and the success stories are very few as compared to junk we have created. Success accomplished to remove some pollution from the beautiful Blue planet.

Key words:

Ghost nets, Microplastic, cosmetics, *Ideonella*

Introduction:

Microbes have been on this planet since azoic era, we are very new species on the planet, but we have very successfully harmed this planet, since last three centuries and now thriving to save our planet. This microbes are of great use to us, since they know to survive better than us in any adverse conditions as there Biotypes that are surviving after hazardous impact are having better modified genetic material to withstand sudden changes to slow changes in nature. Thus, they are generous enough to help us in removing the pollution, that is we label as "Bioremediation". The concept of bioremediation was first used on a large scale in 1972 for the cleaning of Sun Oil pipeline spill at Ambler, Pennsylvania (Kumar et al., 2015). The most common types of bioremediations are microbial bioremediation, phytoremediation, and mycoremediation. Bioremediation is very safe because it uses the same microbes that already naturally occur in soil or water. This process simply adds more of these organisms to those already present. It will always be difficult to obtain 'miracle microorganisms' or the hyper accumulative plants needed in bioremediation processes.

1) Accumulation of plastic:

For many countries, the rainy season is the plastic season. The banks of rivers are washed clean but all the plastic debris is on the to the sea, some of it is deposited on beaches. . Plastic production is booming since the 1950s, as plastic is non-biodegradable, there is a build-up or accumulation of plastic as more and more is released into the environment. "mycoremediation" (Andrady et al., 2011; Cole et al., 2011) is big threat, broken-down pieces of larger plastic debris, tire and clothing wear are the largest source of secondary microplastics in water. Machine washing and drying clothes is also a major source of microplastics pollution which is difficult to control. Five kilograms of synthetic clothing releases an average of nine million microfibers that are carried down the drain with the rinse water. Dozens of other types of microplastics in their products. Polyethylene is found in various cosmetics such as eyeliners, mascara, lipsticks, powders and skincare products (Tanaka and Takada, 2016). The only guarantee for customers that a care product is truly free from all microplastics and nano plastics comes from the brand itself.

Remedial methods:

The discovery, by a team co-led by Prof John McGeehan, is another leap towards beating plastic waste. The scientists who re-engineered the plastic-eating enzyme PETase have now created an enzyme 'cocktail' which can digest plastic up to six times faster. The formation of Microplastics or nanoplastic particles takes place due to the biodegradation of macroplastics in each ecosystem (Richardson and Ternes, 2017). Various biological factors are involved and influenced by the multistage process (Pauli et al., 2017). Depending upon temperature, pH, surface roughness, electrostatic interaction, surface hydrophobicity has the potential to form bacteriological biofilms (Rummel et al.,2017). Under harsh conditions, several microorganisms change their morphology. Around 32 bacterial species are known to break down plastic Due to the high molecular weight of plastic material, it shows a hydrophobic nature on the surface and due to these bacteria show a difficulty in breaking it down into small molecules. The bacterium Ideonella sakaiensis (Yoshida et al., 2016). degrades PET by producing two enzymes performing each their own task. The first enzyme, PETase, cuts the polyester polymer of which PET is constructed into smaller pieces. This enzyme converts the MHET into ethylene glycol and TPA. Under precisely controlled laboratory conditions, the colony in about six weeks completely degrade a sample PET sheet.

2) Ghost net:

Until the early 1960s, natural materials such as cotton and hemp were commonly used. With the advent of polyamide- based nylon after World War II, synthetic fibers quickly replaced natural materials (von Brandt, 1984). The excellent fishing performance, high strength and low price of synthetic materials contributed to the development of worldwide gillnet and driftnet fisheries (Anonymous, 1990; Wright & Doulman, 1991; Richards, 1994). Abandoned, lost or otherwise discarded fishing gear (GHOST NETS) from net fisheries entangle and kill larger marine animals, sea birds, disturb spawning grounds and smother habitats, thereby serving as major hazards and a long- term threat in marine environments (Matsuoka, Nakashima & Nagasawa, 2005; Wilcox et al., 2013). Nylon nets, loose their ghost fishing capacity when they degrade, but they do not disappear from the system. They may degrade into smaller plastic particles that may continue to disturb various processes in the marine ecosystem (Moore, 2008).

Remediation:

In Korea (Republic), a manufacturing method for fishing nets has recently been developed that uses biodegradable resin which can be decomposed by microbial action (bacteria and fungi) after a certain amount of time underwater (Kim, Park & Lee, 2014b,c).

The biodegradable monofilament was produced using a resin blend of 82% polybutylene succinate (PBS) and 18% polybutylene adipate- co- terephthalate (PBAT). Since biodegradable materials are finally degraded to carbon dioxide, methane and water, they do not have any additional impact on marine ecosystems once they have degraded (Tokiwa et al., 2009; Kim et al., 2015,), however 42 months are taken for biodegrading, material is expensive.

Conclusion: All the techniques of bioremediation are very expensive, will require lot of efforts to find the miracle microbe. Bioremediation is a waste management technique that relies totally upon type of microorganisms involved and their biological activity to interact with the environmental factors thereby causing change in the physical and chemical conditions of hazardous waste and finally convert it into comparably less toxic or even nontoxic products. Tones of such magic microbes will be required to disintegrate the amount of waste generated from last two centuries. It will better we use less of plastic.

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Excess Gibb's free energy of activation, excess specific acoustic impedence, for binary mixtures of Diethyl Oxalate + Ethers

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Abstract

Densities (ρ), viscosities (η) and speeds of sound (u) of binary mixtures of diethyl oxalate with ethers (butyl vinyl ether, diisopropyl ether, anisole and dibutyl ether) at (303.15,308.15 and 313.15) K were measured over the entire composition range. From these experimental data excess Gibb's free energy of activation of viscous flow ΔG^{*E}, excess specific acoustic impedence Z^E were calculated. These quantities have been fitted to the Redlich-Kister polynomial equation and results analysed in terms of molecular interactions and structural effects. The obtained data for viscosity were fitted to Mc-Allister(4-body) viscosity model and speeds of sound for Junjie's model

Introduction

Thermodynamics plays an important role in numerous industries in the design of separation equipment and process as well as for product design and optimizing formulations. Complex polar and associating molecules are present in many applications for which different type of thermodynamic and transport properties need to be known over wide ranges of temperature and pressure. Diethyl oxalate is a polar simple aliphatic ester that is full of benefits and find many industrial applications. It is a chemical intermediate used in various dyes. It can be used as a solvent for a number of synthetic and natural resins. It is used as cost effective additive based in the dye sensitized solar cells. Likewise, ethers are used for many purposes and find good applications in chemical engineering areas. Due to fast changing trends of the environmental concerns the need for oxygenated compounds (ethers) are becoming important because of diminishing petroleum reserves and increasing air pollution. The oxygenated fuels are mostly octane enhancers and reduce carbon monoxide emission.

Experimental

All chemicals utilized in this study were of analytical grade supplied by Sigma-Aldrich. The binary liquid mixtures were prepared by mixing known masses of pure liquids in airtight stoppered bottles. Densities of pure and their binary mixtures were determined using a density meter (DDM -2910 Rudolph Research Analytical). Viscosities of the pure liquids and their mixtures were determined by using Ubbelohde viscometer. The speeds of sound of pure liquids and liquid mixtures were determined by using a single-crystal variable path interferometer (model F-81) supplied by Mittal Enterprises, New Delhi, India operating at frequency of 2 MHz.

Result and Discussion

The dependence of excess Gibb's free energy of activation of viscous flow ΔG^{*E} on the mole fraction of diethyl oxalate xi, is shown in Fig 1. A perusal of these isotherms reveals that for diethyl oxalate+ butyl vinyl ether, diisopropyl ether, dibutyl ether the ΔG^{*E} values are negative while for diethyl oxalate+ anisole ΔG^{*E} value is positive across the composition range at all the studied temperatures.

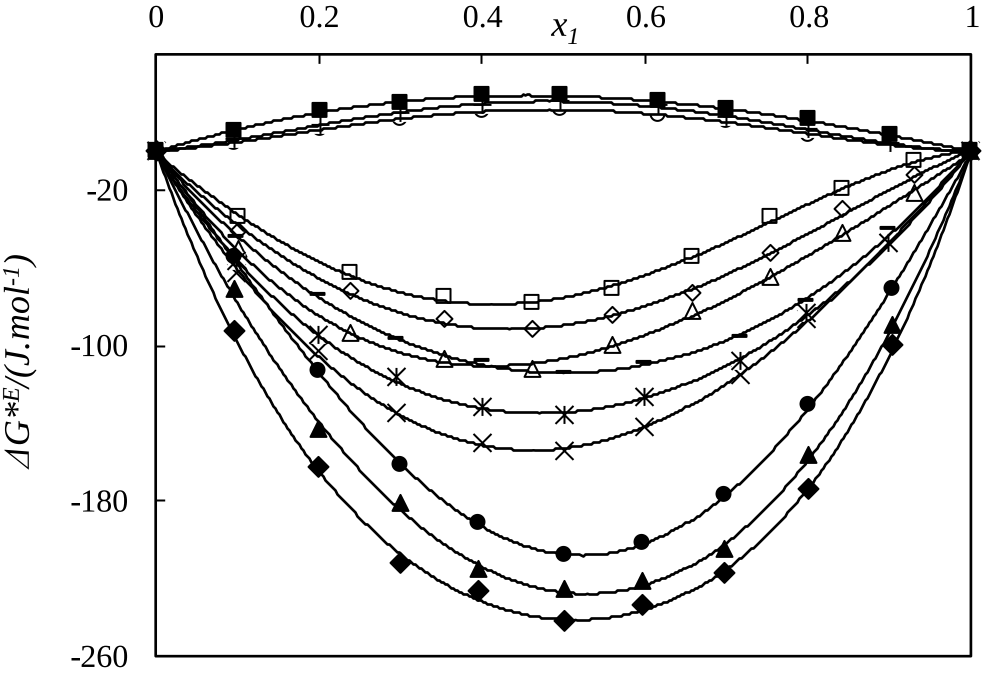

Figure 1. Excess Gibb's Energy (ΔG^{*E}) Vs Mole fraction (x_1) for the binary mixtures of
Diethyl oxalate + Butyl vinyl ether at (□,303.15; ◊,308.15; Δ,313.15)K,
Diethyl oxalate+ Diisopropyl ether at (×, 303.15 ; ж, 308.15 ; ▬,313.15) K
Diethyl oxalate + Anisole at (O, 303.15; +, 308.15; ■, 313.15) K
Diethyl oxalate + Dibutyl ether at (■,303.15; ▲,308.15; ●, 313.15) K

The observed negative ΔG^{*E} value may be due to strong interaction between two component molecules.

The variation in excess specific acoustic impedence Z^E Vs mole fraction (x_1) of diethyl oxalate is plotted in Figure 2. It is observed that for the system anisole the Z^E is completely positive over the entire composition range while for all the remaining systems (butyl vinyl ether, diisopropyl ether and dibutyl ether) the Z^E values bare completely negative. The system diisopropyl ether exhibit large negative values while for dibutyl ether these values are less negative. The negative values of Z^E at the studied temperatures for (Diisopropyl ether, dibutyl ether and butyl vinyl ether) suggest the presence of weak interactions between the component molecules of the mixtures.

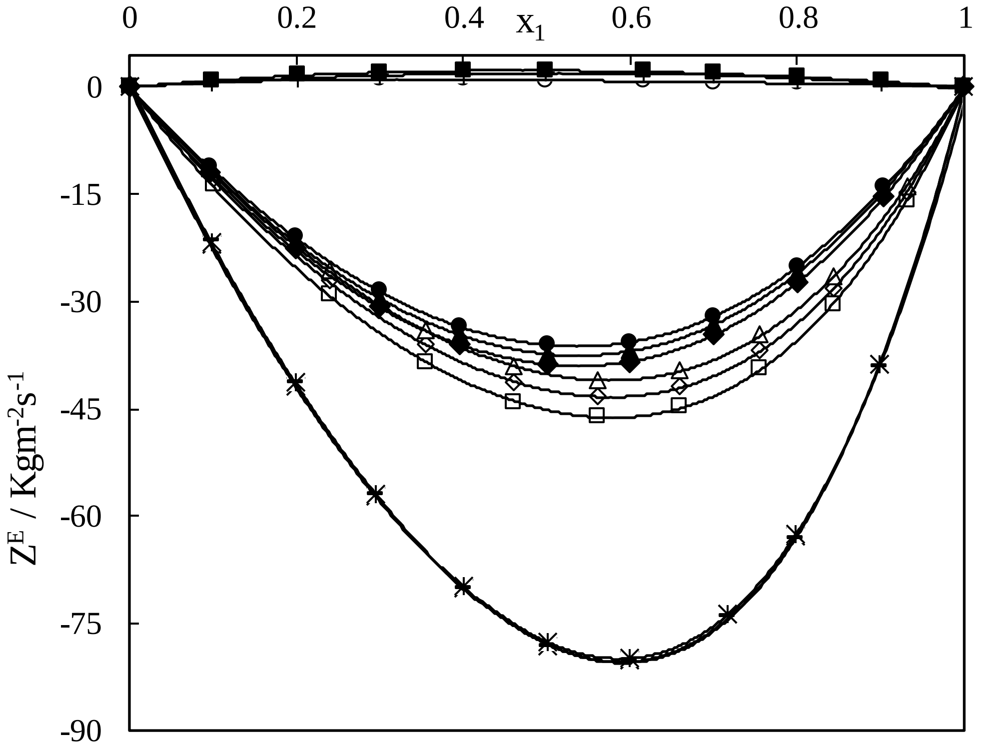

Figure 2. Curves of excess acoustic impedence(Z^E)Vs mole fraction(x_1) for the binary mixtures of,
Diethyl oxalate+ Butyl Vinyl ether at (□, 303.15 ;◊, 308.15 ;Δ,313.15)K,
Diethyl oxalate+Diisopropyl ether at (×,303.15; ж, 308.15 ; ▬,313.15)K,
Diethyl oxalate+Anisole at(O, 303.15 ; +, 308.15; ■,313.15)K,
Diethyl oxalate+ DiButyl ether (♦,303.15;▲, 308.15 ; ●, 313.15)K

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SECTION III

REPORTS

Report

THE FIRST PREPARATORY WORKSHOP OF NATIONAL ONLINE CONFERENCE ON

“ADVANCES IN CHEMICAL SCIENCES AND SUSTAINABLE DEVELOPMENT”

(6th February 2021)

The First Preparatory Workshop of National Conference on- “**Advances in Chemical Sciences and Sustainable Development**” Organised by Department of Chemistry, VPM’s B. N. Bandodkar College of Science, (Autonomous) Thane in collaboration with Department of Chemistry, Dr. Homi Bhabha State University, Institute of Science, Mumbai.

The workshop was held on **6th February 2021** and inaugurated virtually at the hand of **Prof (Dr.) Shivram S. Garje,** Associate Dean, Science and Technology University of Mumbai, Mumbai. The workshop comprised in 3 sessions, **113** participants attended this workshop. All participants were joined google Link https://meet.google.com/hcw-eqyk-igu and it was streamed on you tube link - https://youtu.be/GLoVF6M137Y. **Views on youtube are 832**. The workshop was fully handle by our UG and PG volunteers.

The **first session** began with the virtual welcome to the guest by head of the chemistry department **Dr. D.R. Ambavadekar**. He gave information about infrastructural facility available in our college and showered inspirational words for the audience.

Dr.Gayatri Barbade , Head, Department of Chemistry , Dr. Homi Baba State University The Institute of Science , Mumbai has introduced the function and history of institute of science which is formally known as Royal *Institute of Science (RIS) was established by Royal Charter*.

By virtual offering garland to Late Dr. V N Bedekar, **Opening Remark** of first preparatory workshop of National Conference was delivered by **Dr. A S. Goswami-Giri,** Associate professor in Chemistry and IQAC Coordinator, VPMs B N Bandodkar College of Science, (Autonomous) Thane. She explained that college conducts two preparatory workshops before any conference for the young buddies’. These workshop assistances to inculcate scientific values and analytical thinking among the students. She said, our management leadership believes in our brain which has a capacity for learning that is virtually limitless which makes every human a potential genius. Hence to fulfill it college drives various activities. She also explained thrust areas in chemical sciences which is the theme of the conference on **April 9 & 10 2021**.

Capt. (Dr). Moses Kolet, I/C Principal, VPMs B N Bandodkar College of Science, (Autonomous) Thane was addressed the gathering and welcomed to all virtual delegates. He also appreciated cooperation and collaboration extended by Dr. Homi Baba State University, The Institute of Science, Mumbai. He also appealed to all , to participate in upcoming second preparatory workshop to be held on March 6 and conference on **April, 9 & 10 2021.**

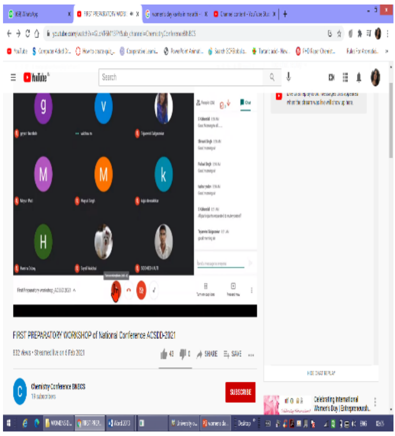
In the **Second session, Prof (Dr.) Shivram S. Garje**, focused the Materials for Environmental Remediation and Sustainable Development. Sir has explained History of human, scientific development, synthetic rubber, first crystal, fullerene, industrial evolution. He also clarified that the Minamata disease case in relation to genetic damage and its journey towards the research (Hg, cobalt containing enzyme) bio methylation reaction. He also focused on Covid-19 and sustainable development nanomaterials, conductors, semiconductors, renewable resources, supercapacitors and its applications.

Dr. Anand Malankar, Research and Development, Head, IFFCO-Personal Care Division, Dubai, delivered talk on Synthesis of compounds having fragrance and flavor with its application technology. Marvelously he explained -Brand , products, types of perfumery industries, hairs care skin care, oral care ,fragrance and deodorant, soap shower gels , color cosmetics, perfume oil, and their manufacturing process, various ingredients used in it, quality of materials characteristic. He contributed the idea about market size of materials for business beneficial.

In the **third session,** virtual tour of institutional activities, followed by six **papers were presented by young budding scientist on pharmaceutical and color chemistry in relation to sustainable development.**

The participant's doubts and queries were addressed by the speakers in **question- Answer session** which was handled by Dr. Rohini Kharade, VPMs B N Bandodkar College of Science, (Autonomous) Thane and Dr.Vikas Bangde , Dr. Homi Bhabha State University, Institute of Science, Mumbai.

The workshop was concluded with vote of thanks by Dr..Sandeep.K. Kahandal organizing secretary of the conference.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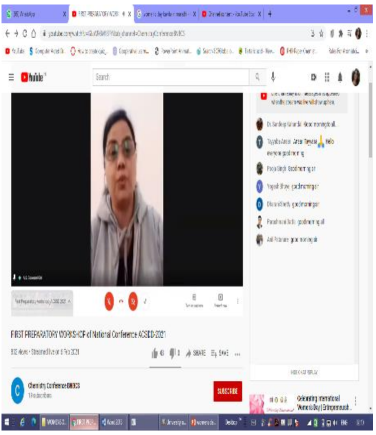
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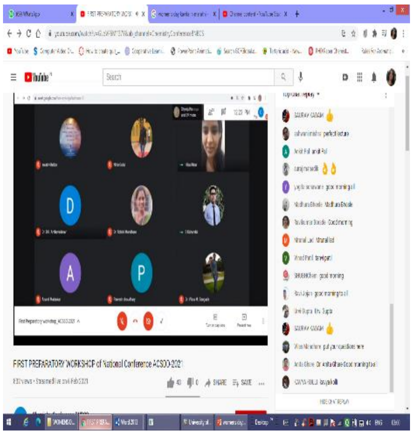
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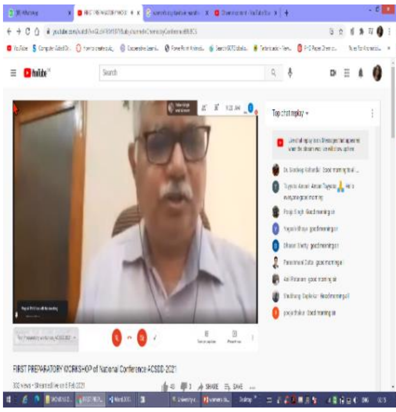
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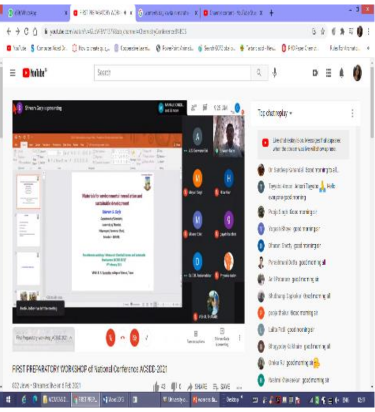
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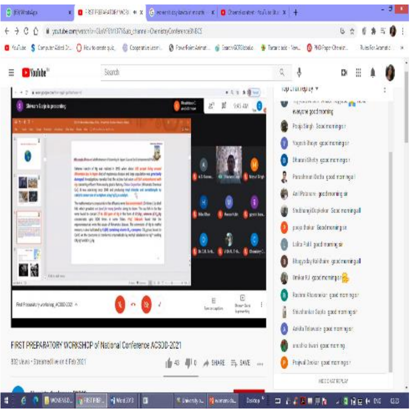
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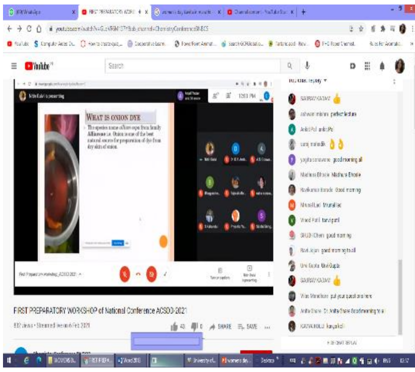
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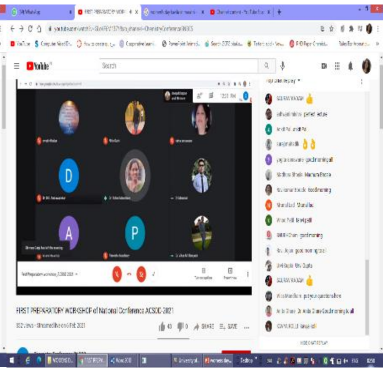
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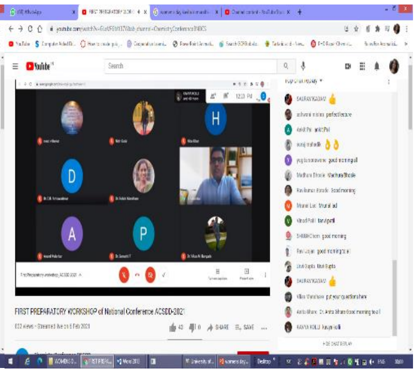

FIRST PREPARATORY WORKSHOP of National Conference ACSSD-2021

Report

THE SECOND PREPARATORY WORKSHOP OF NATIONAL ONLINE CONFERENCE ON "ADVANCES IN CHEMICAL SCIENCES AND SUSTAINABLE DEVELOPMENT"

(6th March 2021)

The Second Preparatory Workshop of National Conference on "**Advances in Chemical Sciences and Sustainable Development**" Organised by Department of Chemistry, VPM's B. N. Bandodkar College of Science, (Autonomous) Thane in collaboration with Department of Chemistry, Dr. Homi Bhabha State University, Institute of Science, Mumbai.

The workshop was held on **6th March 2021** and inaugurated virtually at the hand of **Prof. Yuvraj S. Malaghe, Joint Director, Mumbai division and Head, Department of Chemistry, The Institute of Science, Mumbai, Dr. Homi Bhabha State University.**

The workshop comprised in 3 sessions, **93** participants attended this workshop. All participants were joined google Link https://meet.google.com/aws-zifz-ieu and it was streamed on you tube link - https://www.youtube.com/watch?v=Y3ENKk05jts. **Views on youtube are 700**. The workshop was fully handled by our UG and PG volunteers.

The **first session** began with the virtual welcome to the guest by head of the chemistry department **Dr. D.R. Ambavadekar**. He gave information about infrastructural facility available in our college and showered inspirational words for the audience.

Dr.Gayatri Barbade , Head, Department of Chemistry , Dr. Homi Baba State University The Institute of Science , Mumbai has introduced the function and history of institute of science which is formally known as Royal Institute of Science (RIS) was established by Royal Charter.

By virtual offering garland to Late Dr. V N Bedekar, **Opening Remark** of second preparatory workshop of National Conference was delivered by **Dr. A S. Goswami-Giri,** Associate professor in Chemistry and IQAC Coordinator, VPMs B N Bandodkar College of Science, (Autonomous) Thane. She explained that college conducts two preparatory workshops before any conference for the young buddies'. These workshop assistances to inculcate scientific values and analytical thinking among the students. She said, our management leadership believes in our brain which has a capacity for learning that is virtually limitless which makes every human a potential genius. Hence to fulfill it college drives various activities. She also explained thrust areas in chemical sciences which is the theme of the conference on **April 9 & 10 2021**.

Capt.(Dr). Moses Kolet, I/C Principal, VPMs B N Bandodkar College of Science, (Autonomous) Thane was addressed the gathering and welcomed to all virtual delegates. He also appreciated cooperation and collaboration extended by Dr. Homi Baba State University, The Institute of Science, Mumbai. He also appealed to all to participate in conference which is going to be held on **April, 9 & 10 2021.**

In the **Second session,** Dr. Hemantkumar S.Chandak, Associate Professor in Chemistry and Coordinator IQAC G.S.Science, Arts and Commerce College Khamgaon, Buldhana. Sir has many publications in internationally reputed research journal. He focused on the Green synthesis of heterocyclic compounds using MCR and catalysis.

Prof. S. T. Mhaske, FMASc. Head, Department of Polymer and Surface Engineering Institute of Chemical Technology, Mumbai. He has published many research papers in recognized international journals. Sir has done many minor and major research projects. In the workshop he talked on Sustainability of Flexible Polymer Packaging. Also about its application, Trends and current challenges in that field.

In the **third session,** virtual tour of institutional activities, followed by paper presentation session in that students presented papers **on pharmaceutical and color chemistry in relation to sustainable development.**

The participant’s doubts and queries were addressed by the speakers in **question- Answer session** which was handled by Dr. Rohini Kharade, VPMs B N Bandodkar College of Science, (Autonomous) Thane and Dr.Vikas Bangde , Dr. Homi Bhabha State University, Institute of Science, Mumbai.

The workshop was concluded with vote of thanks by Drs. Sushma Ambadekar, Dr. Homi Bhabha State University, Institute of Science, Mumbai

VPM's B N BANDODKAR COLLEGE OF SCIENCE, THANE

Department of Chemistry

Report on Virtual Poster Presentation

(31st March, 2021)

The workshop on '***How to prepare poster and Virtual poster presentation'*** was held on **31st March, 2021** with the view of students should present their research papers in the Online National Conference- Advances in Chemical Science and Sustainable Development (ASSD-2021) organized by Department of Chemistry.

The Co-convener and Associate professor Dr. A. S.Goswami-Giri along with Mr. Nitin Gulvi, Assistant professor, conducted the workshop for students to create a poster for effective communication their message to the target audience. This workshop was for all the participants making the attendees aware of poster and poster presentation, the initial hurdle that most students face while trying to make poster.

Dr. Goswami-Giri explained, the communication can be done for any message to reach audience. All minute's details including- bullet points, colours, font size, gif, effects, required matter on slide etc. which is needed for perfect poster was explained was by giving examples. She prepared simple slide to explain every things precisely. She also shared her experience related to virtual poster presentation. It evidently showed the amount of attention and smartness one needs to put in to message full in virtual poster. She showed different forms of samples copies of posters.

Strategies for catching the audience attention towards the poster. The session was attended by 24 student poster presenters for the national conference. Overall the workshop was very informative and skilled full for the students.

Report

NATIONAL ONLINE CONFERENCE ON "ADVANCES IN CHEMICAL SCIENCES AND SUSTAINABLE DEVELOPMENT"

(9th and 10th April 2021)

Department of Chemistry, VPM's B. N. Bandodkar College of Science, Thane in collaboration with Department of Chemistry, The Institute of Science, Dr. Homi Bhabha State University, Mumbai conducted a two-day National Conference on ***Advances in Chemical Sciences and Sustainable Development*** on April 9 & 10, 2021. The aim of this conference was to bring together scientists, professors, researchers and research scholars to exchange and share their experiences to highlight the recent developments in the field of sustainable chemistry.

Day 1 April 9 2021

The program was inaugurated virtually at the hands of Chief Guest **Dr. Anthony Melvin Crasto** followed by virtual tour of both the institutes.

Dr. D.R. Ambavadekar, Head and Vice-Principal of VPM's B. N. Bandodkar College of Science, Thane and Convener, who welcomed the participants, guests and provided information about Bandodkar College of science (Autonomous) Thane-1.

It was followed by **Dr. Jairam M. Khobragade**, Director of The Institute of Science, Mumbai who informed the participants about the glorious past of The Institute of Science.

This was then proceeded by Convener in Chief and Chair of the conference, **Capt.(Dr). Moses Kolet,** I/C Principal, VPMs B N Bandodkar College of Science, (Autonomous) Thane. Sir was virtually lightened the lamp on the photo of Dr V N Bedekar and addressed the gathering. He also greeted to all virtual delegates and congratulated to organising committee, convener and Co-convener. He also appreciated cooperation and collaboration extended by Dr. Homi Baba State University, The Institute of Science, Mumbai. Sir enlightened about the journey of college and motivated all participants.

By virtual offering garland to Late Dr. V N Bedekar, **Opening Remark** of National Conference was delivered by **Dr. A S. Goswami-Giri, Co-convener, Associate** professor in Chemistry and IQAC Coordinator, VPMs B N Bandodkar College of Science, (Autonomous) Thane. She explained that college conducts two preparatory workshops before any conference for the young buddies'. These workshop assist to inculcate scientific values and analytical thinking among the students. She said, our management leadership believes in our brain which has a capacity for learning that is virtually limitless which makes every human a potential genius. Hence to fulfil it college drives various activities. She also explained thrust areas in chemical sciences which is the theme of the conference.

The paper to be presented in the conference in the ISBN proceeding soft format was released at the hand of Chief Guest **Dr. Anthony Melvin Crasto**, Principal Scientist at Glenmark Pharmaceuticals Ltd. Sir stressed on the importance of green chemistry for sustainable development.

The keynote address of conference was delivered by **Prof. Sanjio S. Zade**, Professor of Chemical Sciences (DCS) at IISER, Kolkata. He stress 0n *Thiophene containing ladder-type next-gen organic semiconductors.* He said about molecular shape, orbital engineering and crustal engineering. Synthesis of Teatra-substituted thiophene and its changing equivalence differ in production. He stress upon - Stille coupling. He also informed about Pi conjugated system in organic electronic devices and general use of organic semiconductors.

The role of chemistry in the field of nanotechnology was explained by Prof. Vivek Polshettiwar, Associate Professor in the Department of Chemical Sciences at TIFR, Mumbai. He delivered a talk on the topic: *Nanochemistry for Sustainable Development.* He explained the challenges of 21st century which can be solved by using "*Carbon Capture and Conversion to Chemicals* "I He gave example of Haber-Bosch ammonia synthesis, earth energy budget, climate change due to excessive CO2 level which most serious problem. He exhibited modelling of high surface area porous material.

Dr. Amit Zodge, R & D, Manager of Spice King Holland (SKH), Netherlands delivered a talk on topic: *The Green Solvent-Supercritical CO2 technology for Sustainable Chemistry*. Role of CO2 in bio extraction, Super Critical Fluid (SFC) *He* explained the Resolution of alpha methoxyphenyl acetic acid with R-ethyl cyclohexylethyl amine amines and its distereoisomeric properties are same and outcome of it for the development of semiconductors. He also stressed on the single crystal study and its outcome.

The paper presentation session encompassed with 11 scientific research papers;

Day was concluded with Dr. Gayatri Barabde, Convener and Head of the Chemistry department at The Institute of Science, Mumbai as the Convener concluded the conference and wished the participants for their future research.

Day 2, April 10 2021

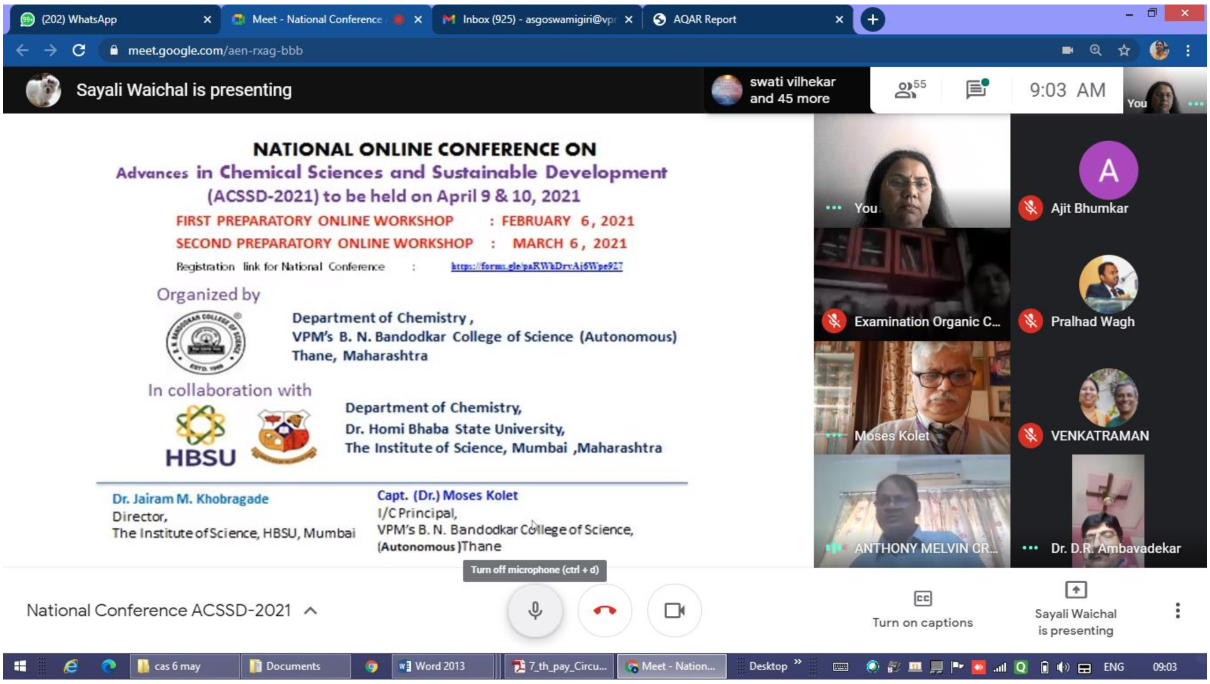
The program was started with talk of Dr**. Muralidhar N. Ingale**, Director of Reynish Pharmachem Pvt. Ltd, Vadodhara. He focused on - *Strategic approaches for optimizing performance and streamlining operations to foster quality and growth for the chemical industry.*

Prof. Rajendra N. Shirsat, Professor of Physical Chemistry, Department of Chemistry, Goa University. He delivered a talk on the topic - *Topography of Molecular Electrostatic Potential.*

Third session was a poster presentation. Dr. Raju Mane was chairperson for this session. Participants put forward poster presentations on various topics related to sustainable chemistry The Valedictory function was ceremoniously conducted by **Prof. A.D. Sawant**, Former Vice Chancellor, University of Rajasthan, Jaipur; Former Joint Director of Higher Education, Mumbai ; Former Pro Vice Chancellor, University of Mumbai

The conference served as a common platform for participation of experts from Industry, Academia and Research organizations who provided insights into the current scenario and technological advancements in green chemistry.

Vote of thanks was given by Dr. Vikas M. Bangade. National Conference was concluded with Glimpses of the conference, followed by National anthem.



NATIONAL ONLINE CONFERENCE ON

Advances in Chemical Sciences and Sustainable Development

(ACSSD-2021) to be held on April 9 & 10, 2021

FIRST PREPARATORY ONLINE WORKSHOP : FEBRUARY 6, 2021

SECOND PREPARATORY ONLINE WORKSHOP : MARCH 6, 2021

Registration link for National Conference : https://forms.gle/paRWhDrvAj6Wpe9Z7

Organized by

Department of Chemistry,
VPM's B. N. Bandodkar College of Science (Autonomous)
Thane, Maharashtra

In collaboration with

Department of Chemistry,
Dr. Homi Bhaba State University,
The Institute of Science, Mumbai ,Maharashtra

Dr. Jairam M. Khobragade
Director,
The Institute of Science, HBSU, Mumbai

Capt. (Dr.) Moses Kolet
I/C Principal,
VPM's B. N. Bandodkar College of Science,
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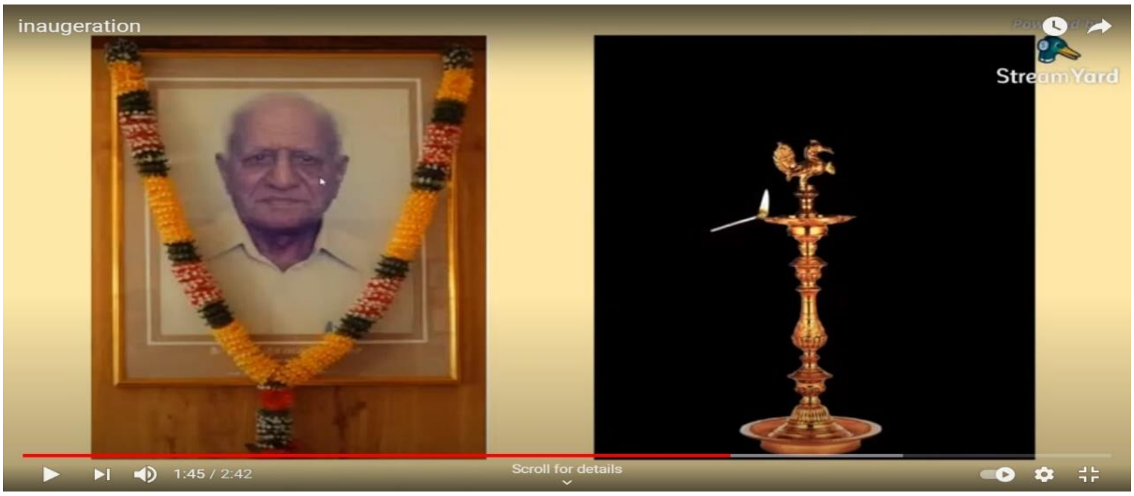

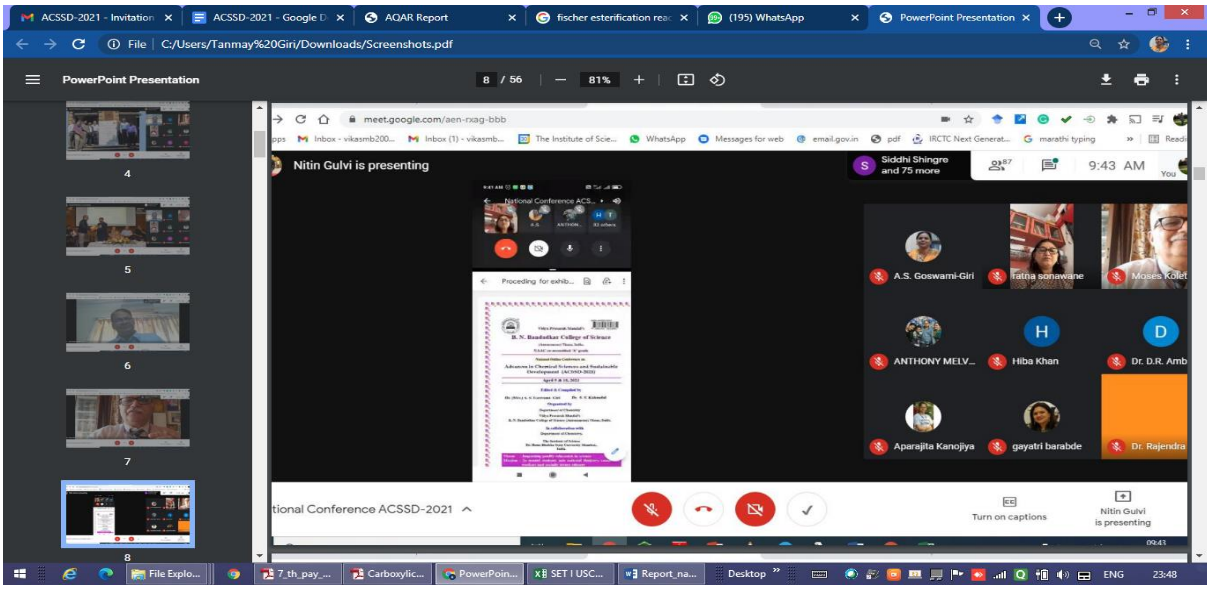

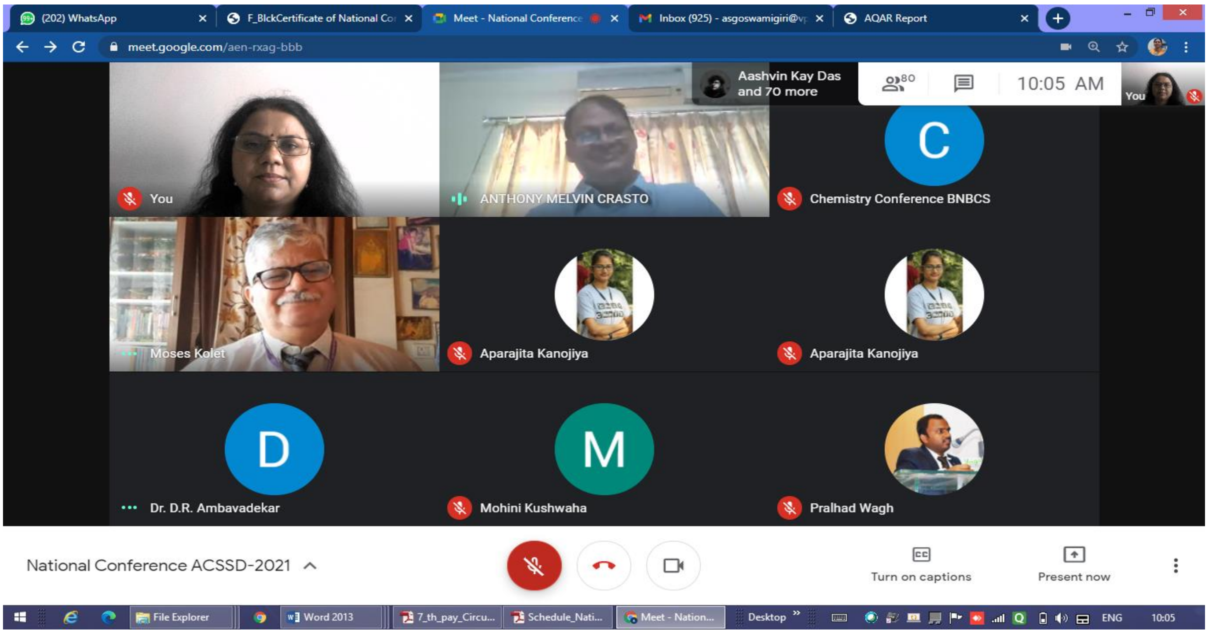
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