

1st International Industrial Chemistry Conference (IICC – 2021)

26-28th February, 2021



Organized by:

**DEPARTMENT OF CHEMISTRY, NED
UNIVERSITY OF ENGINEERING &
TECHNOLOGY, PAKISTAN**



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BOOK OF ABSTRACTS
1st International Industrial
Chemistry Conference
(IICC-2021)
26-28th February, 2021

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Message Of Vice Chancellor, NED University of Engineering & Technology



It is my great pleasure to warmly welcome you to the 1st International Industrial Chemistry Conference (IICC-2021). As a Patron of Conference, I would like to congratulate the organizing committee for organizing conference scheduled for February 26-28th, 2021 at NED University of Engineering & Technology, Karachi.

The three days virtual conference is not only designed to provide and share the latest information and developments on industrial chemistry and related disciplines, but it will also contribute to motivate engagement, networking, and collaboration among researchers from renowned universities and professionals from industry for sustainable future and humanity friendly environment.

I am confident that you will enjoy a stimulating conference here in NEDUET, which will deliberate and discuss all the different facets of industrial chemistry. Your presence and participation will help contribute to this vibrancy and enrich discussions around the theme, developing professional knowledge exchange, insights and collaborations that will lead to a better, healthier, merrier world.

My best wishes for an effective, fruitful and successful conference.

Dr. Sarosh Hashmat Lodi

Vice Chancellor & Conference Patron,
NED University of Engineering & Technology



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Message Of Pro-Vice Chancellor, NED University of Engineering & Technology



I am honored and delighted to welcome you to the International Industrial Chemistry Conference (IICC-2021) and warmly acknowledge the organizers of the conference. This conference is particularly timely in view of the tremendous importance of science and technology in achieving the Sustainable Development Goals (SDGs).

Improvements in the industrial sectors are essential to achieve these goals and thus improve human and environmental health. I hope, this conference will facilitate networking, information exchange and collaboration within and among the private sector, the public sector and civil society; something of great importance to achieve sustainable food security and industrial goals in a globalized world.

I hope you have a good time and opportunity to connect with expertise from scientific community and influential entrepreneurs through their lectures and presentations and will also put forward many thought-provoking strategies on the traditional and advanced technologies in the field of industrial chemistry and related disciplines.

I hope that the experiences of this event will be engraved in your memory.

Have a great conference time.

Dr. Muhammad Tufail

Pro Vice Chancellor & Conference Co-Patron,
NED University of Engineering & Technology



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Message Of Dean - ISH NED University of Engineering & Technology



As Dean and Conference Co-Patron, on behalf of the Faculty of Information Science and Humanities (ISH) at NED University of Engineering & Technology, I am delighted to welcome all participants to the forthcoming 1st International Industrial Chemistry Conference (IICC-2021) scheduled to be held at NED University of Engineering & Technology in Karachi, Pakistan on 26-28th February, 2021.

The conference is organized around the major theme “Industrial Chemistry towards Sustainable Future: Growing Together”. I hope that this unique international conference will provide our participants with a truly transformative experience through a variety of knowledge and perspectives so that the complex problems within and among the industrial sector, the public sector and civil society can be improved.

I am confident that over these three days, new partnerships, stronger alliances and even more cooperative relationships will result. I hope IICC-2021 Conference will continue to play its pivotal role in future as well by encouraging and attracting quality research in a variety of key areas pertaining to industrial chemistry and related disciplines.

Dr. Noman Ahmed

Dean ISH & Dean AMS & Conference Co-Patron,
NED University of Engineering & Technology



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Message Of Chairperson – Department of Chemistry NED University of Engineering & Technology



On behalf of the organizing committee, we look forward to welcome you to the 1st International Industrial Chemistry Conference (IICC-2021) at NED University of Engineering & Technology, Karachi from 26-28th February, 2021.

In the present global pandemic, Department of Chemistry, NEDUET has decided to host this conference in a virtual, on-line format and highlight the latest in global industrial chemistry research and development. The 1stIICC-2021 is bringing hundreds of participants and eminent invited speakers across the world from academia and industry, giving them opportunities to share and collaborate the advancement in industrial chemistry research. Hence, we are looking forward to positive outcomes for local Pakistani academia-industrial researchers and new global partners.

The tremendous logistical demands of bringing all of the symposia together, I would like to take this opportunity to thank honorable VC, PVC, Dean (ISH), my departmental faculty and staff, who made it all happen. We are grateful for the generous support from our sponsors whose contributions are valuable to the success of IICC-2021

I am very much pleased to welcome you on-line this year, and look forward to being able to meet you all in person in the future as I think we can all agree, a virtual meeting cannot replace an in-person meeting

Dr. Nuzhat Arshad

Conference Chair, Department of Chemistry,
NED University of Engineering and Technology



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Message Of Conference Secretary

NED University of Engineering & Technology



I would like to personally welcome each of you to the First edition of our conference, “International Industrial Chemistry Conference (IICC-2021); scheduled to be held at NED University of Engineering & Technology in Karachi, Pakistan on 26-28th February, 2021”. It is an exciting time for scientists, academicians, engineering professionals and researchers, to grow and adapt systematic manuscript management, constructive and critical blind review process.

I would like to thank each of you for attending IICC-2021 and bringing your expertise to this grand meeting. As researcher, you have the vision, the knowledge, the resources and the experience to help us pave our way into the future technical activities. Throughout this conference, I request you to stay engaged, keep us proactive and help us bringing out more such events in future.

My personal admiration and gratitude go out to all of you.

Dr. Saeeda Nadir Ali

Conference Secretary

NED University of Engineering & Technology



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Message Of Conference Coordinator

NED University of Engineering & Technology



As a conference coordinator, it is my pleasure to invite you to attend the 1st International Conference on Industrial Chemistry (IICC-2021).

With this not-to-miss program, I am certain that we will meet to discuss the latest advances in industrial chemistry and related disciplines. We are planning to have best oral and poster presentations during the three days, where the thematic talks and the plenary sessions will drive you through the multi sectoral emergence in the Industrial chemistry world. This conference will provide opportunity to scholars, researchers, industrialists to show case and present their ideas, thoughts, developments that could lead to an evocative life in the field of chemistry.

I wish to extend our gratitude to those involved in making this conference a success. To our mother institution, generous sponsors and contributors, and volunteers, for their financial support and mere dedication.

Looking forward to seeing you at IICC-2021 on February 26-28th, 2021.

Dr. Amtul Qayoom

Conference Coordinator

NED University of Engineering & Technology



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COMMITTEES

STEERING COMMITTEE

Dr. Sarosh H. Lodi	Patron, Vice Chancellor, NEDUET
Dr. Muhammad Tufail	Co-Patron, Pro Vice Chancellor, NEDUET
Dr. Noman Ahmed	Co-Patron, Dean ISH, NEDUET
Dr. Nuzhat Arshad	Chairperson, Department of Chemistry, NEDUET

ORGANIZING COMMITTEE

Dr. Saeeda Nadir Ali	Conference Secretary & Associate Professor, NEDUET
Dr. Amtul Qayoom	Conference Coordinator & Associate Professor, NEDUET
Dr. Kashif Ahmed	Associate Professor, NEDUET
Syed Ghazanfar Hussain	Assistant Professor, NEDUET
Mr. Ansar Khan	Assistant Professor, NEDUET
Dr. Anjum Ayub	Assistant Professor, NEDUET
Dr. Shazia Parveen	Assistant Professor, NEDUET
Dr. Syed Farhan Hasany	Assistant Professor, NEDUET
Dr. Rafia Usman Khan	Assistant Professor, NEDUET
Ms. Atia Shamim	Lecturer, NEDUET
Ms. Hira Sultan	Lecturer, NEDUET
Ms. Farhat Ikram	Lecturer, NEDUET
Ms. Ghazala Aftab	Lecturer, NEDUET
Ms. Sadaf Iqbal	Lecturer, NEDUET
Ms. Shumaila Jawed	Teaching Assistant, NEDUET
Ms. Nazish Irfan	IT Manager, NEDUET



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SCIENTIFIC COMMITTEE

Prof. Dr. Syeda Rubina Gillani	University of Engineering & Technology, Lahore, Pakistan
Dr Masooda Qadri	University of Karachi, Pakistan
Dr. Uzma Ashiq	University of Karachi, Pakistan
Dr. Shazia Nisar	University of Karachi, Pakistan
Dr. Hashim Zuberi	Sindh Madressat-ul-Islam University, Pakistan
Dr. Urooj Haroon	Federal Urdu University for Arts Science & Technology, Karachi, Pakistan
Dr. Muhammad Zahid	University of Agriculture, Faisalabad, Pakistan
Dr. Hyder Khuaja	Environmental Health Sciences University at Albany, State University of New York
Dr. Huma Shaikh	University of Sindh, Jamshoro, Pakistan
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Dr. Mahmood Ali	NED University of Engineering & Technology, Pakistan
Dr. Hajra Tahir	University of Karachi, Pakistan
Dr. Waqas Jamil	University of Sindh, Jamshoro, Pakistan
Dr. Noor Akhmazillah Binti Mohd Fauzi	Universiti Tun Hussein Onn Malaysia
Dr. Sonia Zulfiqar	The American University, Cairo
Dr. Malik Dilshad	Institute of Physical Chemistry, Polish Academy of Sciences, Poland



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ABOUT IICC-2021

Department of Chemistry, NED University of Engineering and Technology is pleased to announce commencement of 1st International Industrial Chemistry Conference (IICC-2021), being organized virtually by the Department of Chemistry, NED University of Engineering and Technology, Karachi on 26 -28th February 2021. It is devoted to stimulate engagement, networking and collaboration among researchers from renowned universities, research institutes and professionals from industry to encourage knowledge and technology exchange by sharing strengths for mutual benefit. The conference will contribute in promoting innovation and knowledge sharing on related theme in the country and beyond.

Due to the COVID-19 pandemic, the conference Organizing Committee has planned to conduct an onsite inauguration ceremony of limited guests at Syed Mahmood Alam Auditorium, Main Campus, NED University of Engineering & Technology, Pakistan on 26th February 2021 with strict social distancing. Inauguration ceremony will be followed by virtual keynote, technical and poster presentation sessions. Participating in online technical sessions of IICC-2021 will open the door to researchers in the field through keynote, oral and poster presentations. It will provide an opportunity for a varied community of researchers, industrialists, professors and students to share their research experiences and participate in interactive discussions. Scholars will share their research work or reveal new innovations with a real-time conversation from anywhere in the world.

Conference programme includes 13 keynote talks by 9 international and 4 national level speakers. 09 technical sessions are dedicated to emerging research trends in the field of chemistry such as nanomaterials, pharmaceutical and environmental chemistry, natural products, textile chemistry, catalysts, green approaches, water treatment etc.

Though IICC-2021 is first conference organized by Department of Chemistry, NEDUET, response to “call for papers” is overwhelming. We received more than 150 research abstracts from various countries including Australia, USA, UK, Spain, Morocco, Turkey, Malaysia, Saudi Arabia, Bangladesh, India and Pakistan. Abstract review committee comprising of national and international highly respected researchers shortlisted the abstracts for oral presentation in relevant technical sessions. Besides online oral technical session, posters presentations will also be conducted. It is expected that approximately 1000 participants will be benefited from scientific discourses from IICC-2021 platform. The selected papers will be published in reputable national journals after due peer review process.



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Organizing such a big conference and linking onsite and online audience is not possible without dedicated IT support and monetary input. IT Team of NEDUET is working hard to make it a smooth event and our industrial partners such as Indigo Textiles, Dewan Sugar Mills (Distillery Division) etc. has made it possible by their generously sponsoring the event.

Whole faculty and students of Department of Chemistry are working efficiently to make IICC a memorable learning experience for all participants. It is expected that this IICC-2021 conference will ignite the minds of the participants and delegates to work together to create a sustainable future through innovation in chemistry.



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ABOUT PASTIC



Pakistan Scientific & Technological Information Centre (PASTIC) is a subsidiary organization of Pakistan Science Foundation (PSF), under the umbrella of Ministry of Science and Technology (MoST). PASTIC is a specialized premier organization in the field of S&T information handling and dissemination responsible for catering to information needs of R&D and industrial community across the country. The PASTIC National

Centre is housed at Quaid-e-Azam University Campus, Islamabad having a network of 6 Sub-Centres at Karachi, Lahore, Peshawar, Quetta, Faisalabad and Muzaffarabad.

To begin with PASTIC supported research community across the country when S&T research infrastructure in Pakistan was at a nascent stage and provided facilities including supply of scientific and technical documents, abstracts and indexes, bibliographies, translations, patent information and patent indexes, science reference library service, technological information transfer service, dissemination of computer-based information services, reprographic and publication services.

PASTIC Objectives

- National S&T/R&D Information Repository of indigenous information resources (databases)
- S&T/R&D information dissemination through contemporary reference information tools
- Strengthen National Science Reference Library for resource sharing & Inter-library collaborations (consortium) and empowerment of information professionals.
- Promotion of R&D based industrial development
- Facilitate printing of S&T/R&D Publications
- Capacity/skill development of researchers & entrepreneurs
- Develop collaborations with national and international information networks

PASTIC Activities/Functions

PASTIC Online databases

Pakistan Science Abstracts (PSA): National research published in Pakistani S&T Journals & Conference Proceedings etc.

PakCat: Union online Public Access Catalogue (OPAC) of Books available in Science and technology Libraries of Pakistan.



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DSpace full text digital repository of indigenous S&T literature.
Database of R&D Projects executed in Pakistan & Industry related databases.

S&T Publications

- Pakistan Journal of Computer & Information Systems (PJCIS): A biannual Open Access primary Journal meant for researchers from Computer Science & Engineering, Information & Communication Technologies (ICTs), Information Systems, Library and Information Science.
- Technology Roundup: Publish bi-monthly bulletin by repackaging of latest global Trade and Technology information.
- Union Catalogue: Provide information on research materials (books/journals/conference proceedings/reports, etc.) available in different S&T libraries of Pakistan.
- Directory of Scientific Periodicals of Pakistan: A handy guide of scientific periodicals published in Pakistan.
- Abstract Books of Conferences: PASTIC support publication/printing of Abstract Books organized by various S&T universities (on request).

Promotion of Commercializable Technologies & Industrial Products

Organize STEM and IT Expo to promote local Research and Development, SMEs, technologies/products/services/industrial R&D challenges/issues as well as empowering youth and general public on new and faster ways of delivering and accessing information.

National Science Reference Library Facility

A state of the art Traditional Library facilitating the researcher through following services: Reference & Referral Services; Reader Service; Internet Service, Journal Listings; Photocopying & Scanning Services.

Human Resource Development (Capacity Building)

Organize Seminars/Workshops /Trainings/ for capacity building of:

Young Researchers on Data Analysis and bibliographic citation Tools (SPSS, EndNote, Mendeley)

Women Entrepreneurs on e-marketing and e business skills

Library Professionals on Library Information Management Tools & techniques (Koha, D-space etc)

Researchers and entrepreneurs on Intellectual Property Rights, Media Information Literacy



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IICC-2021 & SUSTAINABLE DEVELOPMENT GOALS

The Sustainable Development Goals (SDGs), also known as the Global Goals, were adopted by all United Nations Member States in 2015 as a universal call to action to end poverty, protect the planet and ensure that all people enjoy peace and prosperity by 2030. The 2030 Agenda was adopted in 2015. The Agenda's 17 SDGs and their associated 169 targets aim at stimulating action over the next 15 years in areas of critical importance for humanity and the planet. They are integrated and indivisible and balance the three dimensions of sustainable development: the economic, social and environmental. The 17 SDGs are integrated that is, they recognize that action in one area will affect outcomes in others, and that development must balance social, economic and environmental sustainability. Everyone is needed to reach these ambitious targets. The creativity, knowhow, technology and financial resources from all of society is necessary to achieve the SDGs in every context. Achieving the SDGs requires the partnership of governments, private sector, civil society and citizens alike to make sure we leave a better planet for future generations. This 1st International Industrial Chemistry Conference (IICC-2021) aims to stimulate the collaboration and networking between researchers, policy makers and stakeholders targeting at how and which of the SDG's will be addressed. This conference will provide them a better platform to show how their research will contribute to achieve SDG's of 2030.





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CONFERENCE PROGRAMME

Day-1			
Inaugural Ceremony			
Key Note Session 01			
Key Note Session 02			
Key Note Session 03			
Key Note Session 04			
Technical Session 01	Technical Session 02	Technical Session 03	Poster Display
Analytical Techniques and Pharmaceutical Analysis	Nanomaterials for Environment	Chemistry for Industrial Sustainability-I	
Day-2			
Key Note Session 05			
Key Note Session 06			
Key Note Session 07			
Technical Session 04	Technical Session 05	Technical Session 06	Poster Display
Recent Catalysts for Environment	Clean Energy & Waste as Valuable Resource	Chemistry for Industrial Sustainability-II	
Key Note Session 08			
Key Note Session 09			
Technical Session 07	Technical Session 08	Technical Session 09	Poster Display
Latest Research in Medicinal Chemistry	Trends in Synthetic Chemistry	Chemistry for Industrial Sustainability-III	
Day-3			
Key Note Session 10			
Key Note Session 11			
Key Note Session 12			
Key Note Session 13			
Closing Ceremony			

** Detailed conference programme is available on conference website.*



**IICC-2021
MAIN SPEAKERS
(BIOGRAPHIES)**



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Dr. Mohammad Nahid Siddiqui

Prof. Dr. Mohammad Nahid Siddiqui received his Ph.D. in Chemistry from Heriot-Watt University, Edinburgh, UK and MS degrees from KFUPM, Dhahran, Saudi Arabia and AMU, Aligarh India. Dr. Siddiqui is a Professor of Chemistry at King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, Saudi Arabia. He has published more than 185 papers in Journals & conferences, one book and one book chapter. He holds 20 US patents issued by USPTO, USA. Completed more than 30 research projects funded by KACST/KFUPM. He is member of American Chemical Society. His areas of research included but not limited to developing porous materials, polymer composites, and chemistry of asphaltene, chemical recycling of waste plastics, water purification, aging and polymer modification of asphalts.



Dr. Syeda Rubina Gilani

Prof. Dr. Syeda Rubina Gilani completed her Post Doc. in Inorganic/Analytical Chemistry in 2008 from Queen's University Kingston, Ontario Canada. Her field of research was Novel Ru Complex of Methyl diphenylcyclopentadienylide. She has over 30 years of research/teaching experience. Her research interest includes Environmental Toxicology, Toxicology w.r.t. human health, Phytomedicine chemistry, Functional Food Chemistry, Biosynthesis of Metal NANO Particles and Renewable Energy Resources.





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Dr. Sarfaraz Niazi



Dr. Sarfaraz Niazi, Adjunct Professor at the University of Illinois, University of Houston and several other universities is an author of 50+ major books in the field of pharmaceutical biotechnology, cGMP manufacturing and formulations; he holds 50+ US patents on biotechnology and new drugs; he has established the first biosimilar company in the US and taken several biological products through regulatory approvals. He is CEO of RNA Therapeutics, Inc., developing both preventive and therapeutic vaccines, besides developing biosimilar. He is also an advisor to regulatory agencies worldwide including the FDA and also to several heads of state on healthcare programs including Joe Biden team.

Dr. Zyta Maria Ziora



Dr. Zyta Ziora received Ph.D. (Wroclaw University of Science & Technology, Poland) in chemistry and has wide range of experience in medicinal chemistry, including development of antimalarial therapeutics (the University of Montpellier, France), enzyme inhibitors and drug candidates against Alzheimer disease (Kyoto Pharmaceutical University, Japan). Her research time is currently dedicated mainly to projects devoted to the modification of existing antibiotics, and complexing them with other antimicrobial agents, e.g. metal ions, to produce more potent alternatives able to overcome the drug resistance of superbugs.



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Dr. Ian Watson

Dr. Ian Watson obtained his first degree in Applied Physics, and a PhD in Laser Systems then began to research the effects of laser radiation on bacteria and microorganisms in the early 90s. Dr. Ian Watson research interests range from exploiting bio-energy and microalgae, laser asteroid detection and laser and combined systems for inactivation of microorganisms. Areas permeating each theme are complex experimentation, real time detection, monitoring and control of processes.



Dr. Muhammad Saleem

Dr. Muhammad Saleem has specialization in Water Resources & Environmental Engineering. At present, he is serving at Jubail University College (JUC), Royal Commission of Jubail, Saudi Arabia. He is member of various national and international organizations including Associate Member, ASCE and NACE International. Before joining JUC, he worked as Principal Engineer, at Karachi Institute of Power Engineering, Karachi. Dr. Saleem has published more than **100 papers** in reputable national and international journals and conferences. He has organized several workshops, conferences and seminars. Several students completed their Master's and PhD under his supervision. Dr. Saleem is also a **technical reviewer** of more than 45 international journals. He is **Editor** of six journals and **Associate Editor** of an international journal.





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Dr. Muhammad Akram Shaikh



Prof. Dr. Muhammad Akram Shaikh is working as Director General in Pakistan Scientific & Technology Information Centre (PASTIC), a subsidiary of Pakistan Science Foundation under Ministry of Science & Technology. He is author of more than 40 journal/conference papers of national/international repute. In addition, he is involved as editor/ co-editor/ reviewer of national/international journals and Session chair/ PC member of national/international conferences at various national/international forums. His research areas of interest include Knowledge Engineering, Scientific & Technological Databases, Information Processing, Data Mining & Data Warehousing, Big Data & Analytics, Software Engineering, Automation & Control, Social Networks, Virtual Reality and Graphics.

Dr. Muhammad Farooq Wahab



Dr. M. Farooq Wahab is a Research Engineering Scientist at the University of Texas at Arlington. He did his Ph.D. from the University of Alberta, Canada, he worked as a Postdoctoral fellow with Dr. Armstrong and assisted him in his start-up company. His research interests include new detection technologies and signal processing. He serves on the editorial advisory board of *Chromatographia*. Dr. Wahab was selected among “Top 40 under 40 Analytical Chemists” by the Analytical Scientist Magazine. He received the “Young Investigator Award” from the Chinese American Chromatography Association in Pittcon in 2019. The Journal of Separation Science has included him in Emerging Thought Leaders in Separation Science in 2020.



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Dr. Fernando Bimbela

Dr. Fernando was a member of the Thermochemical Processes Group from 2004 to 2014, a research group from the Aragon Institute for Engineering Research (I3A) in aforementioned university. In 2015, he got a position as a lecturer in the Public University of Navarra (UPNa, Pamplona, Spain), where he is currently working as a Senior lecturer at the Sciences Department. Since 2015, he is also a member of the Chemical Reactors and Processes for the Valorization of Renewable Resources group (QuiProVal), led by Prof. Dr. Luis Gandía.



Dr. Adnan Javed Pirzada

Dr. Adnan Javed has sixteen years of experience in the field of process engineering during which he has been able to have hands on experience of installation & commissioning of Ethyl Alcohol Manufacturing Unit & Bio-Gas Manufacturing Unit in collaboration with French Engineers. Trouble shootings and modifications in steam boilers, steam turbines has been an important area of his filed experience. He has received on the job training for S.A.P and participated in Performance Management Workshop in Singapore from internationally acclaimed trainer Mr. Harold Monty Sacher.





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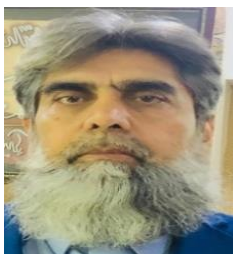


Mr. Syed Iqbal A. Kidwai



Mr. Kidwai holds two Masters, a MS in Development Administration, from Michigan USA and a Masters in Economics at the University of Punjab, Lahore and Diplomas in planning & management from Harvard University Boston, the Netherlands, and Germany. He has practical work experience of 30+ years in the key areas of Strategic Planning, Public Administration & Management, of providing oversight for training & capacity building, replicating/customizing best practices & innovation for competitiveness & sustainable development. He served in the Pakistan Civil Service on key assignments including deputy commissioner, deputy secretary, project director etc., provided consulting services at UNDP, UNDCP, World Bank, JICA, IUCN, and New-Zealand projects. Currently, he is working as Secretary General/CEO for Pakistan Chemical Manufacturers Association (PCMA) to achieve competitiveness, implementing best practices for chemical industry, including safety & security coordinating with National Authority, Ministries of Foreign Affair, Commerce, Industries, Climate Change, FBR/Finance, Narcotics Control Division of Pakistan & international agencies e.g. OPCW, INTERPOL, The American Chemistry Council, Nitric Acid Climate Action Group and related agencies

Dr. Shahid Afghan



Dr. Afghan is CEO, Sugarcane Res & Dev. Board Govt. of Punjab, Pakistan. He has 30 years of R&D experience in Sugarcane crop production, and project head of Organic production. He is member of 10 national and international scientific societies and has organized six workshops on sugar cane crop and also participated sugarcane crop international conferences in USA, Brazil, Thailand, China, Sri Lanka, South Africa and Mauritius. Dr. Afghan is author of three books and one training manual on sugarcane production technology with more than 100 research papers in open access and impact factor journals in the country and abroad. He has been awarded with four gold medals for best research work on sugarcane crop improvement.

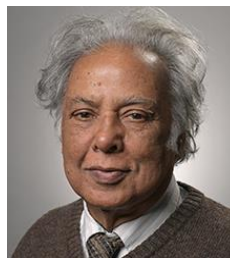


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Dr. Syed Arif Kazmi

Prof. Dr. Kazmi has a Ph.D. in chemistry from Kent State University, Kent, Ohio. He did Post-doctoral research at the University of Maryland (College Park) and University of Illinois (Urbana-Champaign). He has taught at Hunter College of City University of New York, Rutgers University (NJ), Georgia State University, University of Karachi (Pakistan) in the Department of Chemistry and the International Center for Chemical and Biological Sciences (ICCBS, Karachi). He retired as Professor and Chairman of Department of Chemistry, University of Karachi. He taught graduate level courses in inorganic reaction mechanisms and bioinorganic chemistry, guided over a dozen Ph.D. dissertations and has contributed 72 research articles in peer-reviewed journals.



Dr. Saqib Nasir

Dr. Saqib Nasir holds Ph.D. in the field of low-rank coal (lignite) processing and utilization technologies in collaboration with Monash Energy Chemistry Group, Monash University, Melbourne, Australia. He has 18 years of professional experience in research and development while serve various public and private organizations. Presently, he is working as Principal Scientific Officer at Pakistan Science Foundation (PSF). He is author / co-author of 23 research papers published in peer-reviewed Fuel, Fuel Processing Technology and Environmental Engineering Journals. He is renowned invited speaker in 43 national and international conferences, workshops, and seminars.

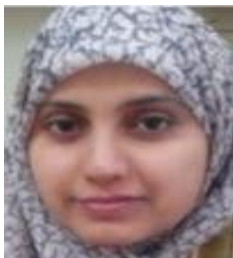




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Dr. Nuzhat Arshad



Dr. Nuzhat Arshad did her Masters with Gold medal distinction from University of Karachi in 2002. Dr. Nuzhat completed her PhD studies in 2009 from Karl Franzens University of Graz, Austria on microwave assisted organic synthesis of bioactive heterocycles. Dr. Nuzhat is HEC approved PhD supervisor and reviewer in the field of chemistry. She has won several HEC funded projects and has supervised several research students. Dr.

Nuzhat has several collaborative projects with various universities including Federal Urdu University, Bahria University and University of Karachi. She is co-authors of high impact publications in the field of Chemistry. She has honor to report novel BIQUIP ligands and several medicinally important heterocyclic compounds.

Dr. Mehmood Ali



He holds a Ph.D. degree in Mechanical Engineering from the University of Glasgow, Scotland, UK. He received his Bachelors and Masters of Engineering, from NED University in Mechanical and Environmental Engineering, respectively. His areas of research and expertise include Biodiesel Production, Combustion and Emission characteristics of Biodiesel Blends, Thermochemical Treatment of Biomass, Solar Biomass Drying System and Bioenergy Generation from Agricultural Residues.



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Dr. Huma Shaikh

Dr. Huma Shaikh is working as an Assistant Professor in National Center of Excellence in Analytical Chemistry, University of Sindh, Jamshoro. She was awarded Ph.D. degree in Analytical Chemistry in the year 2015. She has good expertise in synthesis of materials mainly nanomaterials, polymeric membranes, graphene and its derivatives, etc. She is working on the utilization of said materials for the development of new analytical procedures and decontamination of environment. She has 20 international publications and has produced 08 M.Phil. Scholars.



Dr. Urooj Haroon

Dr. Urooj Haroon holds Ph.D.in Chemistry from University of Karachi. She is working as Assistant Professor in the Department of Chemistry, Federal Urdu University for Arts Science and Technology. She has 19 publications to her credit, a chapter in a book, 7 BS research students and two PhD students. Dr. Haroon is an associate editor of FUUAST Journal of Biology and active member of American Chemical Society. Her areas of interest are organic synthetic chemistry, pharmaceutical chemistry, and applications of nanoparticles in medicine and environment.





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Dr. Agha Zeeshan Mirza



Dr. Zeeshan holds Ph.D. in Organic Chemistry, from University of Karachi. During the Ph.D. he worked with Prof. Dr. Joseph Irudayaraj at Purdue University in West Lafayette, Indiana, USA as a Visiting Research Scholar. Later, he joined Intertek Testing Services at Karachi as Research and Development Manager. In 2012, He took a Research Associate position at Umm al Qura University in Makkah, KSA, worked on the Synthesis and Computer-Aided Molecular Drug Design of

Isoxazolidine Nucleosides Derivatives with Potential Anticancer Activities. Dr. Zeeshan's research involves synthesis of biologically active molecules. His most recent work is on Drug Design of bi-functional hybrid agents. He has published 53 peer-reviewed research papers in national and international journals.



**IICC-2021
KEYNOTE
ABSTRACTS**



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IICC21- KN-02	Potential of Ethyl Alcohol Manufacturing for Professional Engineers and Analytical Experts in Pakistan and its Significance in Pakistan's Economy and Global Economy <u>Adnan Javed Pirzada</u>
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KEY NOTE NO.	TITLES
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IICC21- KN-09	Sugarcane Biofuels and Bioenergy Production in Pakistan: Current Scenario, Potential, and Future Avenues <u>Shahid Afghan</u>
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IICC21-KN-01



How can We Protect Our Skin Against Microbes?

Zyta Maria Ziora^{1*}

*¹Institute for Molecular Bioscience, The University of Queensland, St Lucia,
QLD, Australia*

**E-mail: z.ziora@uq.edu.au*

The spread of resistant bacteria, leading to untreatable infections, is a major public health concern. The antibiotic discovery to combat these pathogens has recently significantly slowed down causing major health concerns worldwide. The twenty-first century is a renaissance of the metals, as one of the possible alternatives to treat diseases caused by multidrug-resistant bacteria. Metals have been used as antimicrobial agents since antiquity, but throughout most of the history their modes of action have remained unclear. Recent studies indicate that different metals cause discrete and distinct types of injuries to microbial cells as a result of oxidative stress, protein dysfunction, or membrane damage.

Today, antimicrobial metal compounds have a multitude of applications in industry, agriculture and healthcare. Silver is the most promising among them due to its multidirectional activity. Therefore, development of silver resistant bacteria is very difficult and requires multiple mutations in the cell.

Additionally, natural products, such as berry fruits and citrus have been used as alternative sources for curative treatment due to their presence of bioactive molecules possessing antimicrobial, antioxidant, antitumor and anti-inflammatory effects, and providing complete biodegradability, environmentally friendly productions, with fewer side effects, lower toxicity, and lower expenses. Therefore, the design of novel metallodrugs, as a hybrid complexes of nature-derived nature ceuticals and silver, is highly promising strategy to develop effective and safe treatment against variety of human pathogens.

Keywords: Antimicrobial, Bioactive, Antitumor.



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IICC21-KN-02



Potential of Ethyl Alcohol Manufacturing for Professional Engineers and Analytical Experts in Pakistan and it's Significance in Pakistan's Economy and Global Economy

Adnan Javed Pirzada^{1*}

¹General Manager, Dewan Distillery Division, Dewan Sugar Mills

*Email: adnan.pirzada@yousufdewan.com

The feedstock for Pakistan Ethanol is Molasses derived from Sugar cane. Sugarcane is an important industrial and cash crop in Pakistan. The statistics show that sugar cane is grown on an area of 1.1 million hectares. Total production of Molasses in last year was 2.25 Million MT. Hence the emergence of this new sector in the manufacturing segment has huge potential for professional engineers, analytical experts, and technological experts. It has become a significant source to bring foreign exchange into the national exchequer through its exports from Pakistan to across the globe. For manufacturing of ethyl alcohol, diluted molasses with developed culture of yeast and nutrients is fed to fermentation tanks for the production of ethyl alcohol. The reaction takes approximately 40 hours to complete and all the sugar content is converted into ethyl alcohol and CO₂ which leaves the tanks from the top. This entire process is very hygiene sensitive and involves lots of research and analytics for having maximum process efficiencies and consistent product quality. Pakistan is one of the Quality suppliers of ethanol in the world and has exported approximately 400,000 MT in last year and maximum export from Pakistan in one year were 653,000 MT in 2017~18. Last 05 years scenario of ethanol exports in small packs (ISO Tanks and FCLs) have increased year on year basis. In 2021 it is estimated that globe production could reach about 110 billion liters. The surging demand to produce ethanol from sugar is likely to provide opportunities for the market studied during the forecast period. It is expected that the food-grade Ethanol demand scenario remains firm across the world, because of an increase in Health & Hygiene Products.

Keywords: Pollasses, Sugar, Ethenolscope, Global Economy.



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IICC21-KN-03



Synthetic mRNA Vaccine Development

Sarfaraz K. Niazi^{1*}

¹*University of Illinois, USA*

**Email: sniazi3@uic.com*

Now after 225 years of first vaccine use, we have a synthetic nucleotide vaccine that is readily and quickly manufactured to handle pandemics and provide a new therapeutic tool. Nucleotide vaccines, DNA or RNA-based, are the newest types of vaccines; the first mRNA vaccine was approved in 2020 to prevent COVID-19. Therapeutic vaccination, a form of immunomodulation that assists in the treatment of infectious diseases, cancers and autoimmune disorder like diabetes that will soon become available. An mRNA vaccine or mRNA (messenger RNA) vaccine inserts mRNA in lipid nanoparticles, a sequence codes for antigens and identical proteins resembling those of the pathogen leading to translation by the host cells to produce the encoded antigens, which then stimulate the body's adaptive immune system to produce antibodies against the pathogen. Another form of the mRNA vaccination is when the mRNA encodes for a fully human IgG antibody. In this form, the mRNA codes for antibodies that are identical or resembling those of the antibodies found in a patient with a prior history of potent immunity. I am presenting details of mRNA technology that can be readily deployed by developing countries to make the vaccines to meet domestic needs

Keywords: Vaccines, mRNA, DNA, Synthetic vaccine, Pandemic response, COVID-19.



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IICC21-KN-04



Global Solutions from Bio Refineries to Mitigate Climate Chaos

Ian Watson^{1*}

¹*James Watt School of Engineering, University of Glasgow, UK*

**Email: ian.watson@glasgow.ac.uk*

The world is in climate chaos, largely driven by emissions from energy production from fossil fuels. Whilst there is immediate urgency to reduce carbon emissions, there is a growing demand for energy. Meeting this demand through renewable energy sources such as solar and wind partly addresses the problem, but fails to address their intermittent nature and the need for materials and products that stem from the petroleum industry. Biorefineries, exploiting biomass feedstock for energy production and higher value products, offer a sustainable approach that can deliver energy, power and replacement products from the fossil fuel industry such as bioplastics, new products relating to pharmaceutical and nutrition and allows energy on demand and natural storage in the feedstock. Importantly, biorefineries allow the potential for bioenergy carbon capture and sequestration (BECCS), offering the only global route towards truly negative emissions. To meet global targets on emissions to reduce temperature rise, it is crucial that such technology is implemented at scale. The work will address the problems associated with this approach, how systems can be implemented and some of the underlying research that is being doing to enable this vision to become a reality.

Keywords: Bio Refineries, BECCS, Gasification, Pyrolysis, Microalgae.



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IICC21-KN-05



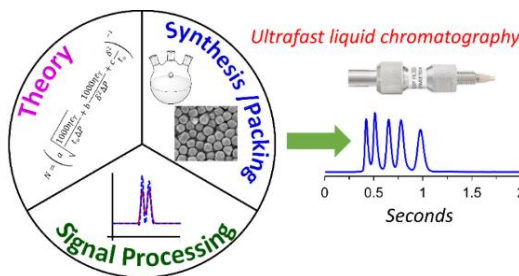
Chiral and Achiral Separations at Sensor Speeds - Greener Alternatives to Toxic Solvents in Separation Science

M. Farooq Wahab^{1*}, Daniel W. Armstrong¹

¹Department of Chemistry & Biochemistry, University of Texas at Arlington,
Texas, 76019, USA

*E-mail: mfwahab@uta.edu

Chemical sensors have the virtue of speed for single component analysis. Sensors produce the analyte-specific signal in a few seconds. Unfortunately, sensors are heavily affected by the sample matrix. Chromatographic analysis has the power of removing interferences and is compatible with multiple analytes. However, the speed of traditional UHPLC analyses is not even close to sensors. In this presentation, approaches for ultrafast chiral chromatography are discussed. A variety of macrocyclic glycopeptides were bonded on core-shell particles for chiral separations. The high efficiencies, selectivity, and low back pressures in short-packed columns were very advantageous for separations in the sub-second range. Custom made beds were compacted at very high pressures (13,000 psi). Ultrafast LC saves time, solvents and increases the throughput in biomedical and pharmaceutical research. In the end, alternatives to toxic and expensive solvents currently used in chiral analysis using sub/supercritical CO₂ are discussed.



Keywords: Chiral, Achiral,
Sensor, UHPLC.



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IICC21-KN-06



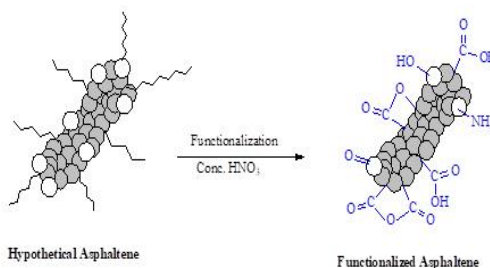
Synthesis of Active Carbonaceous Material from the Functionalization of Asphaltene for Industrial and Environmental Applications

Mohammad Nahid Siddiqui^{1*}

¹Department of Chemistry, King Fahd University of Petroleum and Minerals,
Dhahran 31261, Saudi Arabia

*E-mail:mnahid@kfupm.edu.sa

Consumption of crude oil as a fuel and energy source is being continuously increasing due to fast-paced developments. The major portion of the crude oil is converted into fuel using refining and cracking processes. Asphaltene is one of the undesired components of the crude oil that is the most troublemaker in refining and cracking processes. Asphaltene causes precipitation and depositions in crude oil transporting pipes triggering a reduced flow of the oil, which leads to severe blockage problems. Besides, asphaltenes can form sludge and poison or deactivate the upgrading and refining catalysts leading to reduced efficiency. The asphaltene is an n-alkane insoluble compound having complex chemical structures. We have studied the chemistry of asphaltene extensively and reported that asphaltene is mainly composed of fused aromatic rings bearing alicyclic and aliphatic groups including some heteroatoms and metals. In our work, the asphaltenes were extracted from crude oil and functionalized using nitric acid which developed –COOH, –C=O, –OH, and other functional groups. The functionalized asphaltene was used as an effective and efficient adsorbent for the removal of toxic metal ions and organic pollutants from water. Secondly, functionalized asphaltene was also used as fillers in several thermoplastics leading to enhanced mechanical strength properties.



Keywords: Crude oil, Asphaltene, Functionalization, Adsorbent, Fillers.



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IICC21-KN-07



Active Edible Coatings with Extract of Green Apple (*Malus Pumila*) Peels to Prolong the Shelf Life of the Fruit

Prof. Dr. Syeda Rubina Gilani^{1*}

¹*Department of Chemistry, University of Engineering & Technology Lahore*

**Email: drsrobina@uet.edu.pk*

The use of plastic packaging materials and petroleum-derived plastics produced severe environmental issues, along with oxidation, it is one of the main reasons of quality loss in foodstuffs. For alternate feasible solutions, biodegradable/edible coating for food products is the better choice and the harmful impacts can be delayed by using the active coating containing antioxidants. Active coating innovation is intended to prolong the shelf life of food, sustaining the sensory quality, antimicrobial, nutritional properties, and safety attributes. Green apple containing the high levels of antioxidants and polyphenols which provide protection against cancer is an incredible source of essential vitamins, nutrients for humans. It is susceptible to browning and uses to control gas exchange and moisture transfer. Edible coatings are prepared by making the solution of CMC with water and the apple peel's juice. Apple peel's juice is centrifuged and added to the CMC solution in different concentrations. A homogenous mixture is then applied on apples and Petri dishes and was placed in the oven for 24 hours at 37⁰ C.

Different characterization like anti-microbial, measuring of phenolic contents, FTIR, UV-Spectroscopy, SEM, XRD, and goniometry of these coatings was carried out. These coatings are incorporated with several food additives to enhance food texture, flavor, and color. Food-grade bio macromolecules, in addition to fruits and vegetables, are used for edible packaging having suitable physical-mechanical properties as well as unique sensory and nutritional characteristics.

Keywords: *Malus Pumila*, Antioxidant, Polyphenols.



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IICC21-KN-08



Syngas Production by Catalytic Processing of Methane-Rich Streams: Catalytic Partial Oxidation of Methane and Biogas Reforming.

Fernando Bimbela^{1*}

¹Andrea Navarro-Puyuelo, Ainara Moral, Inés Reyero, Luis M. Gandía, Grupo de Reactores Químicos y Procesos para la Valorización de Recursos Renovables, Institute for Advanced Materials and Mathematics (InaMat²), Department of Sciences, Universidad Pública de Navarra, Pamplona, Spain

**E-mail: fernando.bimbela@unavarra.es*

Gas-to-liquid technologies (GTL) have reached full-scale technology readiness levels, thus enabling for the transformation of methane-rich streams into valuable chemicals and synthetic fuels. In this sense, GTL technologies represent a promising alternative to flaring in non-conventional methane sources such as stranded gas, but also a possibility for upgrading biogas obtained in anaerobic fermentation processes. Key to the development of such technologies is the transformation of these methane-rich streams into synthesis gas, raw material for the synthesis of long-chain hydrocarbons in Fischer-Tropsch processes or for producing methanol. Therefore, efficient catalytic processes for producing syngas must rely on the development of highly active catalysts with adequate selectivity to syngas. In addition, the use of structured catalysts is advantageous in these processes because mass and heat transfer are improved, and high methane conversion levels can be attained at very short contact times, which can lead to process intensification and to the development of compact processing units with industrially relevant capacities for syngas production. This talk will briefly cover some of the research activities developed at the UPNA in the last 5 years, and will review the main findings in our works on syngas production by methane catalytic partial oxidation and by biogas reforming.

Keywords: Syngas, Methane conversion, Partial oxidation, Biogas reforming, structured catalytic reactor.



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IICC21-KN-09



Sugarcane Biofuels and Bioenergy Production in Pakistan: Current Scenario, Potential, and Future Avenues

Shahid Afghan^{1*}

¹CEO, Sugar Res. & Dev. Board Punjab, Pakistan

**Email: ceo.srdb@gmail.com*

Sugarcane is one of the major agricultural commodities of Pakistan. The crop is grown on an area of 1.22 million hectares, with a total production of 73.40 million tons. Sugarcane's role has been limited to sugar production in the past; however, it can play significant role toward energy matrix of the country. Being a developing nation of 197 million people, energy demands of the country are sky-high, whereas indigenous energy resources are meager. Pakistan meets its petroleum demands majorly through imports, while the country is also facing power shortage for more than a decade. Hence, sugarcane, as an energy crop, can play significant role in providing bioenergy in the form of ethanol-blended fuels as well as cogenerated electricity. Pakistan State Oil evaluated E10 blend on limited outlets in 2006 followed by its marketing in 2010. Indigenous ethanol production has increased over time because of new taxes on export of molasses. Fuel grade ethanol is also already being produced by some distilleries; nevertheless, these initiatives have not contributed much toward country's energy matrix because of absence of policies requiring ethanol blends at national level till date. Sugarcane sector can also serve for bioelectricity production in Pakistan. The country has potential to engender approximately 3000 MW of electricity from sugarcane. Various economic incentives have been offered to power producing sugar mills; nevertheless, there is need to increase the support, especially regarding financing for upgrading current low-pressure technology of the mills. Since there is scarcity of hydropower in sugarcane crushing season, cane industry can play important role in tackling the energy shortfall of the country in such months. This chapter analyzes the current status and future perspectives of cane-derived fuels and energy production in Pakistan.

Keywords: Bio-Fuels, Bio-Energy, Sugarcane, E-10 Blend, Bio-Electricity.



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IICC21-KN-10



Role & Potential of Chemical Industry in Economic Development of Pakistan: Contribution of Academia Thereof

Iqbal Kidwai^{1*}

¹General Secretary and Chief Executive Officer, Pakistan Chemical and Manufacturing Association Pakistan

**Email: sg@pcma.org.pk*

PCMA is a forward looking, valued and trusted apex body of Pakistan Chemical industry endeavoring to achieve competitiveness through imports substitution and implementing best practices. Impact of chemical industry on global economy is around \$5.7 trillion and continuous investment in R&D is increasing the size of this pie. This sector not only established strong forward and backward linkages but it is also the 4th largest and 3rd fastest sector in international trade. Its impact on local economy is assessed by the fact that chemical industry is the biggest supplier of textile value chain and contributes around PKR 170 Billion in national treasury. In addition, 1 job created in chemical industry supports 7.8 jobs in the country and \$1 generated in chemical sector increases national income by \$4.2. Despite challenging conditions in domestic economy and cut throat competition from regional players, PCMA members are investing in domestic market to convert imported raw material in to value added products. Share of petrochemicals is over 30% in overall chemical import and most of them are have high growth rates therefore establishment of petrochemical crackers with mixed feed options will open new business avenues in domestic and international market. Domestic production of major petrochemicals can substitute \$5 billion import in short run by 2025 while it will taper down (\$8-10 billion) chemical imports bringing it to minimum. Cracker will move down-stream & up-stream chain and huge small, medium & large investment will pour in for mega manufacturing thereby creating export surplus.

Keywords: PCMA, Chemical Industry, Petrochemicals.



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IICC21-KN-11



Synthesis and Importance of Some Bio-Active Hetero Cycles

Nuzhat Arshad^{1*}

¹*Department of Chemistry, Faculty of Information Sciences and Humanities,
NED University of Engineering Technology, Karachi, 75270, Pakistan*

**E-mail: nuzhat@neduet.edu.pk*

Heterocycles are key structural motifs of many of the drugs available on the market today. The ability of heterocycles to employ a wide variety of intermolecular interactions, wide range of ring sizes and broad array of shapes allows them to bind with enzymes in a multitude of ways, resulted in their diverse applications in medicines. Our interest to make contribution in the field of medicinal chemistry enabled us to produce several new heterocyclic compounds/derivatives namely bisquinolone phosphine (BIQUIP)¹, cyclic thioamides², dihydropyrimidine (DHPM)³ and tetrahydro-2H-1,3,5-thiadiazine thione (THTT)⁴. All new heterocyclic compounds were characterized by spectral techniques including ¹H NMR, ¹³C NMR, and Mass Spectroscopy and were also examined for their biological applications.

Keywords: Heterocycles, bisquinolone, cyclic thioamides, thiadiazine thione, medicinal compounds.



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Evaluation of Fruits Peel Extracts as a Green Corrosion Inhibitor for Mild Steel Protection in Acidic Environment

Muhammad Saleem^{1*}, Tariq Saeed²

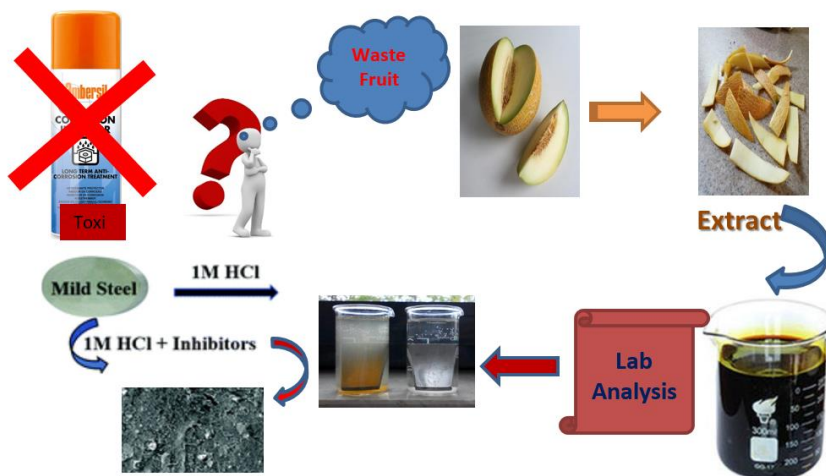
¹Department of Civil Engineering, Jubail University College, Jubail Industrial City 31961, Saudi Arabia

*E-mail: saleemm@ucj.edu.sa

Jubail and Yanbu in the Saudi Arabia are one of the largest industrial setups in the world including petroleum refineries and other production units. Corrosion of metals is a severe problem in these industries which leads to frequent accidents and puts a tremendous economical load. In this study potential of some fruits peels extracts (including Pomegranate, Orange and Sweet Melon) as a green corrosion inhibitor evaluated by weight loss and Potentiodynamic polarization technique. Peel extract of sweet melon (*Cucumis melo* L) in 1M HCl solution were tested at various concentrations (0.05 to 0.5%) and applied to mild-steel coupons in 1M HCl solution. Electrochemical study revealed higher corrosion inhibition efficiency (IE) of the extract (85.52% and 90.12% at low temperature 295K and 318K respectively) showed chemisorption phenomenon. At high temperature it showed physisorption phenomenon (90.12% at 333K) when inhibitor concentration was 0.5%. Various adsorption isotherm were used to fit the data and Langmuir isotherm found to be best-fit models to describe the adsorption phenomena on mild steel. The CR and IE strongly dependent on temperature change. The results obtained from weight loss and Tafel polarization method were proved that the SM is a promising eco-friendly inhibitor for mild steel corrosion.

Keywords: Green corrosion inhibitor, Sweet melon peels (*Cucumis melo* L.), Mild steel, Weight loss, Potentiodynamic study.

Graphical Abstract:





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IICC21-KN-13



Coal Combustion Residual (CCR) Utilization as a Source of Industrial Chemicals

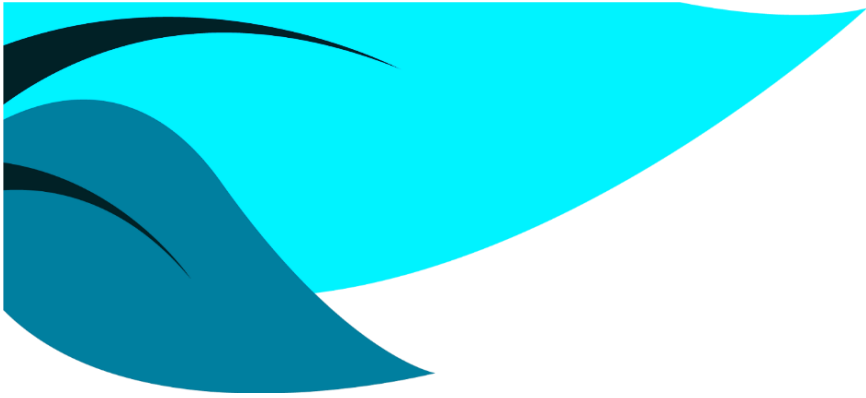
Saqib Nasir^{1*}

*¹Pakistan Science Foundation, Ministry of Science and Technology, 1-
Constitution Avenue, G-5/2,
Islamabad – Pakistan*

**Email: saqibnasir@hotmail.com*

Coal is the major fuel for on-going and future energy projects hence the large scale use of indigenous and imported coal in Pakistan's power sector generate significant quantities of coal combustion residues (CCR). The management and utilization of coal combustion residues (fly ash, bottom ash, chemosphere, conditioned ash, flue gas de-sulphurization and slag) as by-product of coal combustion cycles have become an issue to be solved right away due to environmental concerns and to enhance the productivity and profitability of coal based power generation. This invited talk will highlight the possibilities of using coal combustion residues in engineering, agriculture and allied fields to cater future bulk production of such waste material due to on-going and planned coal-fired power plants in Pakistan. The value added benefits (valorization) of CCR is a global practice to save natural resources, energy, emissions of pollutants to the air, CO₂, SO_x emissions and repository space. The appropriate collection, management and utilization aspects of CCR to explore future opportunities for production of value added industrial chemicals will be likely to discuss in technical talk.

Keywords: Coal; combustion residues; utilization; valorization; industrial products.



Technical Session 01

Analytical Techniques & Pharmaceutical Analysis



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IICC21-O-01	Interaction Studies of Chlorpheniramine Maleate in Aqueous and Aqueous-Alcoholic Systems by Density, Viscosity and HPLC Methods <u>Summyia Masood</u> , Zainab Khan
IICC21-O-02	Advancement in the Development of Heterocyclic Nucleosides for the Different Diseases <u>Agha Zeeshan Mirza</u>
IICC21-O-03	Estimation and Stability Studies of Glibenclamide in Bulk and Pharmaceutical Dosage form <u>Faiza Akhtar</u> , Somia Gul, Wajiha Nasheed, Faizan Baig, Agha Zeeshan Mirza
IICC21-O-04	Interaction of Bioactive Iron with Clinical Chelating Drug, Kojic Acid by Cyclic Voltammetry <u>Kanwal Zahid</u> , Shazia Nisar, Shazia Perveen
IICC21-O-05	Charge Transfer Complexes of Linagliptin with 2,3-dichloro-5,6-dicyano-1,4 Benzoquinone, Chloranilic Acid and Ninhydrin: Experimental and Theoretical Studies <u>Sameera Zaki</u> , Saeeda Nadir Ali, Amtul Qayoom, Rafiq Ahmed
IICC21-O-06	Statistical Experimental Design for Simultaneous Determination of Anti-Diabetic Drugs with NSAID <u>Muhammad Bilal Abbasi</u> , Saeeda Nadir Ali, Amtul Qayoom
IICC21-O-07	Design and Synthesis of Fluoroquinolone Derivatives as Potent α-Glucosidase Inhibitors <u>Aasia Shaheena</u> , Uzma Ashiq, Rifat Ara Jamal, Khalid Mohammed Khan, Sammer Yousuf
IICC21-O-08	Switchable Solvent Based Liquid Phase Microextraction of Rhodamine B Zeliha Erbaş, <u>Mustafa Soylak</u>



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IICC21-O-01



Interaction Studies of Chlorpheniramine Maleate in Aqueous and Aqueous-Alcoholic Systems by Density, Viscosity and HPLC Methods

Summyia Masood^{1*}, Zainab Khan¹

¹*Department of Chemistry, University of Karachi, Karachi-75270, Pakistan*

**E-mail: smasood@uok.edu.pk*

Densities and viscosities of chlorpheniramine maleate in water and also in MeOH/EG aqueous solutions have been measured over a temperature range of 298.15 to 318.15K. Number of several parameters i.e., apparent molar volume (ϕ_v), partial molar volume (ϕ_v^0), Hepler's constant ($\partial\phi_v/\partial P$)_{T,A} (Falkenhagen coefficient) and B (Jones-Dole coefficient) have been calculated by using experimentally measured density and viscosity values. The mentioned calculated parameters were found to be valuable to perceive drug-drug and drug-solvent interactions. Moreover, one of the liquid chromatographic techniques such as RP-HPLC has also been performed and the outcomes supported the conclusion procured from volumetric and viscometric study.

Keywords: Density, Viscosity, RP-HPLC, Drug-solvent interactions, Chlorpheniramine maleate.



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IICC21-O-02



Advancement in the Development of Heterocyclic Nucleosides for the Different Diseases

Agha Zeeshan Mirza^{1*}

¹*Department of Chemistry, Um Al Qura University Makkah, KSA*

**E-mail: azmirza@uqu.edu.sa*

Cancer and viral diseases are widely renowned as significant medical problems. Chemotherapeutic drugs are successful against cancer in several cases and the development of drugs with selective antiviral activity with harmless to host cells is required. Different compounds, including the analogues of natural substances, may be used for these syndromes. Nucleoside, nucleotide, and base analogues have been utilized for decades for the treatment of viral pathogens, neoplasms, and anticancer chemotherapy. Heterocyclic nucleosides analogues have gained a lot of importance in recent years for combating cancer of different types due to diverse nature and possess multiple mechanisms of action. Modified nucleosides are class of drugs widely explored with many of its components already in use in clinical practice. In this context, nucleoside analogues, in which the furanose ring has been replaced by acyclic, carbocyclic, or heterocyclic moieties have attracted increasing interest by virtue of their action as antiviral and/or anticancer agents. This work focuses on the different types of nucleosides and their potential role as anticancer and antiviral agents. It also discusses the nucleoside analogues approved by FDA and in process of approval. The effect of the substitution on the nucleoside analogues and their pharmacological role is also discussed.

Keywords: Heterocyclic nucleoside, Cancer, Isoxazolidine, Chemotherapeutic drugs.



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IICC21-O-03



Estimation and Stability Studies of Glibenclamide in Bulk and Pharmaceutical Dosage Form

**Faiza Akhtar^{1*}, Somia Gul², Wajiha Nasheed³, Faizan Baig⁴,
Agha Zeeshan Mirza⁵**

¹Department of Pharmaceutical Chemistry, Ziauddin University

²Department of Pharmaceutical Chemistry, Jinnah University for Women

³Dow College of Pharmacy, Dow University of Health Sciences

⁴Department of Chemistry, University of Karachi

⁵Department of Chemistry, Um Al Qura University Makkah, KSA

*Email: faiakh90@gmail.com

The purpose of the current study is to develop an easy, sophisticated, and assessable UV method that can be used for routine analysis of glibenclamide. For this reason, a simple inexpensive method was developed and validated as per guidelines for the determination of glibenclamide in bulk and pharmaceutical dosage form using 25% methanolic solution as a solvent. The proposed method is linear ($R^2 > 0.9993$) with the range of 5-50 $\mu\text{g/mL}$, accurate (100.68%), precised intraday (0.322%) and interday (0.932%) and robustness ($\text{RSD} < 2\%$). Stability studies of the drug facilitate to understand the degradation response of the drug and product. In this regard, forced degradation studies of glibenclamide have been conducted. The tested drug was studied under different accelerated environmental conditions. Results revealed degradation of glibenclamide under different accelerated conditions. It is found that in acidic and alkaline environment drug recovered upto 61.90 and more than 90%, respectively. On exposure to UV radiation, 30% (70% recovered) of glibenclamide was degraded. Thermal degradation was 11-19% (89-81% recovered) and in buffers solutions of various pH, degradation was 22%-86.85% (13.15-78% recovered) of the tested drug occurred. The proposed method was also applied for the assay for the pharmaceutical dosage form and found satisfactory results. Results revealed that the proposed study is highly sensitive and can be used for the routine analysis of glibenclamide.

Keywords: Glibenclamide, Stability studies, Forced degradation.



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IICC21-O-04



Interaction of Bioactive Iron with Clinical Chelating Drug, Kojic Acid by Cyclic Voltammetry

Kanwal Zahid¹, Shazia Nisar¹, Shazia Perveen^{2*}

¹Department of Chemistry, University of Karachi, Karachi, 75270, Pakistan.

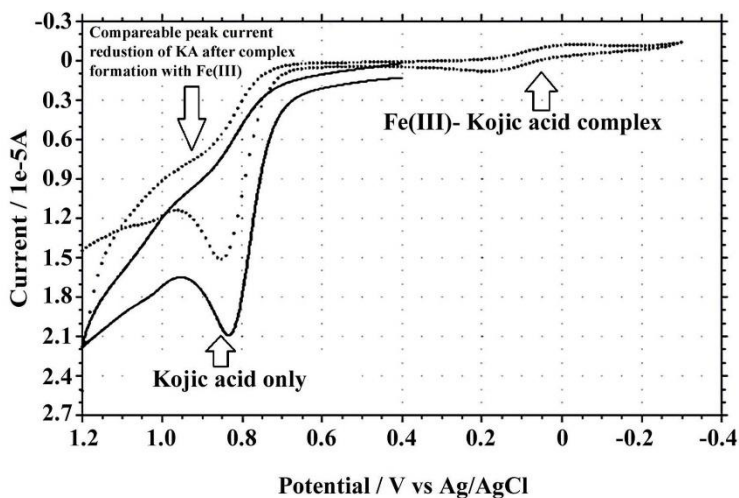
²Department of Chemistry, NED University of Engineering and Technology,
Karachi, 75270, Pakistan.

*E-mail: shaziaperveen@neduet.edu.pk

This study presents spectral and electrochemical studies of Fe(III) complex with Kojic acid (KA) in acetate buffer solution of pH 4.0. UV-Visible analysis shows that three bidentate ligand (L^-) forms neutral complex $[Fe(III) L_3]$ with metal, and it is the dominating existing complex at our experimental condition of pH 4.0. In this work, cyclic voltammetric method is used to evaluate valuable information on redox behavior of Kojic acid in the presence of Fe(III) metal ion. The proposed simple and elegant electrochemical approach is useful for characterization of complex formation as well as for mechanism verification. This study shows that $[Fe(III)L_3]$ complex undergoes one electron reduction by a quasi-reversible, diffusion controlled process. Further to that this one electron reduction of $[Fe(III)L_3]$ complex takes place according to EC mechanism. Electrochemical properties of the complex in comparison of the Fe(II)/Fe(III) redox couple show that complex formation of bioactive metal Fe (III) with KA probably increases the kinetics of electron transfer, which can influence the electron transport chain of biological system. Our FT-IR results show a distinct IR band shifting for carbonyl ($-C=O$) and hydroxyl ($-OH$) group, indicating the chelating moieties of Kojic acid, for the formation of complex at pH 4.0.

Keywords: Bioactive metal, Cyclic voltammetry, FT-IR analysis, Kojic acid, UV/Visible spectroscopy.

Graphical Abstract



Highlights:

- Cyclic voltammetric studies revealed, $[\text{Fe(III)} \text{ L}_3]$ complex undergoes one electron reduction by a quasi-reversible, diffusion controlled process.
- Reduction took place according to EC mechanism.
- Results from UV/visible spectroscopic and FTIR analysis were evident of complex formation at pH 4, so supportive for cyclic voltammetric studies.



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IICC21-O-05



Charge Transfer Complexes of Linagliptin with 2,3-dichloro-5,6-dicyano-1,4-Benzoquinone, Chloranilic Acid and Ninhydrin: Experimental and Theoretical Studies

**Sameera Zaki^{1*}, Saeeda Nadir Ali¹, Amtul Qayoom¹,
Rafiq Ahmed²**

¹Department of Chemistry, NED University of Engineering and Technology,
Karachi, 75270, Pakistan.

²Department of Polymer & Petrochemical Engineering, NED University of
Engineering and Technology, Karachi, 75270, Pakistan.

*Email: sameera.zaki16@gmail.com

Three new intermolecular proton transfer complexes consisting of an antidiabetic drug linagliptin as the electron donor with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone, chloranilic acid and ninhydrin as π -acceptors have been synthesized in methanol. Stoichiometry of complexes was found by utilizing Job's plot method and a ratio of 1:1 was acquired for each complex. The method showed linear calibration curves in the range of 2.84-28.35, 2.36-21.26, 9.45-85.06 μgml^{-1} for DDQ, chloranilic acid and ninhydrin respectively with correlation coefficient greater than 0.997 in each case. The spectral parameters including transition dipole moment, oscillator's strength, molar extinction, ionization potential, resonance energy and thermodynamic parameters, such as association constant and Gibb's free energy were also determined from Benesi-Hildebrand equation. The newly formed charge transfer complexes were characterized by IR spectroscopy, TGA and XRD. The proposed method was successfully applied for the determination of linagliptin in pharmaceutical formulation without interference of excipients.

Keywords: Charge transfer complexes, Linagliptin, DDQ, Chloranilic acid, Ninhydrin, Benesi Hildebrand plot, TGA, XRD



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IICC21-O-06



Statistical Experimental Design for Simultaneous Determination of Anti-Diabetic Drugs with NSAID

Muhammad Bilal Abbasi^{1*}, Saeeda Nadir Ali¹, Amtul Qayoom¹

*¹Department of Chemistry, NED University of Engineering. & Technology,
Karachi, 75270, Pakistan*

**E-mail: bilal20755@gmail.com.*

A precise, accurate, time saving, and robust isocratic RP HPLC method has been developed and validated for simultaneous determination of metformin hydrochloride, empagliflozin and ibuprofen. The stationary phase used was phenomenex octadecyl silyl 250mmx5micron column. Mobile phase was composed of 0.05M phosphate buffer: Methanol in the ratio of 32:68. The retention times were 1.98, 3.79 and 10.30 for metformin hydrochloride, empagliflozin and ibuprofen, respectively. Calibration plots were found to be linear at a range of 70-30 $\mu\text{g/ml}$, 175-325 $\mu\text{g ml}^{-1}$ and 1400-2600 μgml^{-1} for metformin hydrochloride, empagliflozin and ibuprofen respectively. The method was validated for precision, robustness, accuracy, linearity, and sensitivity. Recoveries in percent were found to be close to 100% with minimum variability. Factorial design containing four factors were chosen for screening. Method's system suitability parameters were in range under implement of different robustness parameters. The method may be used in industries for routine analysis.

Keywords: RP HPLC, Metformin, Empagliflozin, Ibuprofen, Factorial design



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IICC21-O-07



Design and Synthesis of Fluoroquinolone Derivatives as Potent α -Glucosidase Inhibitors

Aasia Shaheen¹, Uzma Ashiq^{1*}, Rifat Ara Jamal¹, Khalid Mohammed Khan¹, Sammer Yousuf¹

¹Department of Chemistry, University of Karachi, Karachi-75270, Pakistan

²H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan

*Email: uzma.ashiq@uok.edu.pk

Fluoroquinolones are extensively used in clinical applications as a crucial class of antibacterial medicine and have shown high potential for the treatment of several other diseases. This study is based on synthesis, structure elucidation and biological evaluation of various fluoroquinolone (enoxacin) analogues with electrophilic substitution of aromatic amine moiety of central enoxacin nucleus by benzyl halides. The synthesized derivatives were characterized on the basis of different chemical and physical measurements and structures were elucidated by various spectroscopic techniques (NMR, EI-MS), including elemental (CHN), and X-ray diffraction analysis. Furthermore these compounds were investigated for their potential α -glucosidase inhibition activities and all synthesized analogues of fluoroquinolones were found to exhibit promising inhibition potential of 45.8 ± 0.2 to $74.5 \pm 0.2 \mu\text{M}$ in comparison to IC_{50} value of $425.6 \pm 1.3 \mu\text{M}$ for standard inhibitor of α -glucosidase 1-deoxynojirimycin.

Keywords: Fluoroquinolones, Synthesis, X-ray diffraction, α -glucosidase, Structure activity relationship.



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IICC21-O-08



Switchable Solvent Based Liquid Phase Microextraction of Rhodamine B

Zeliha Erbaş^{1,2*}, Mustafa Soylak^{1,2}

¹ Department of Chemistry, Faculty of Science, Erciyes University, Kayseri, Turkey

² Technology Research and Application Center (TAUM), Erciyes University, Kayseri, 38039, Turkey

*E-mail: erbaszeliha@gmail.com

After enriching with switchable solvent-based liquid phase microextraction, an environmentally friendly method has been developed that includes the accurate and precise determination of Rhodamine B by UV-Vis spectrophotometry. Triethylamine (TEA)/ protonated triethylamine bicarbonate (P-TEA-BC) solvent pair was synthesized and used as switchable solvent in the extraction of Rhodamine B. The effects of analytical parameters affecting extraction efficiency such as pH, switchable solvent and NaOH volume were optimized. Also, the effects of foreign ions were found to be tolerable. Optimum recoveries for Rhodamine B in the sample solution were obtained using 600 μL protonated TEA at pH 4.0. Analytical performance parameters such as the limit of detection (LOD) and pre-concentration factor were determined as 2.96 $\mu\text{g L}^{-1}$ and 25 respectively. Accuracy studies for water samples were checked by addition-recovery studies and recovery in the range of 88-103% was obtained. The developed method has been successfully applied to detect Rhodamine B in environmental water samples.

Keywords: Liquid phase microextraction, Switchable Solvent, Rhodamine B, Spectrophotometric Determination, Water



Technical Session 02

Chemistry for Industrial Sustainability-I



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IICC21-O-09	University–Industry Interaction in Bangladesh: Evolutionary Phases, Forms of Interaction, Benefits, and Barriers <u>Muhammad Jamaluddin Ahmed</u>
IICC21-O-10	Transportation, Economics, Energy Options, Environment and Public Health-Need For a Holistic and Sustainable Approach. Case Study of Karachi. <u>Syed Arif Kazmi</u>
IICC21-O-11	Analytical Chemistry: A Gateway to the Sustainable Industry <u>Huma Shaikh</u>
IICC21-O-12	Sustainable Eco-Friendly Fibers in Textile Industry <u>Syed Muhammad Imtiazuddin</u>
IICC21-O-13	Development and evaluation of herbal formulations against Acne producing microbes M. Hashim Zuberi, Abdullah, <u>Urooj Haroon</u> , Sana Nazeer, Sana Waheed, Sajid Jahangir
IICC21-O-14	Bioplastics: A Green Approach in Materials for Green Environment <u>Nadia Akram</u> , Amina Shafi
IICC21-O-15	Need and Impact of Active Pharmaceutical Ingredient Manufacturing on Economic Development and Healthcare System of Pakistan <u>Tabassum Nusrat</u> , Fareeha Lodhi, Kounain Farheen, Hadiqa Anwar, Nusrat Ghani, Salman Zafar, Muhammad Ali Versiani, Sajid Jahangir, Kehkashan Khan
IICC21-O-16	Synthesis of Salvia plebia Silver Nanoparticles and Their Dyes Degradation Activity Sana Ihsan, <u>Hafiza Salma Bibi</u> , <u>Nargis Jamila</u>



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IICC21-O-09



University–Industry Interaction in Bangladesh: Evolutionary Phases, Forms of Interaction, Benefits, and Barriers

Muhammad Jamaluddin Ahmed^{1*}

¹University of Chittagong, Bangladesh

*Email: pmjahmed55@gmail.com

University–industry interaction (U–I) acquires relevance to countries to the extent that they identify how scientific knowledge produced within universities enhances technological development in firms and facilitates innovations. Universities are invigorated by the possibility of new scientific investigations that these relationships provide. The objective of this article is to analyze the establishment and development of U–I interactions in Bangladesh, of six major universities through evolutionary phases, forms of interaction, benefits, and barriers. A total of in-depth interviews were conducted during the data collection stage. To support the analysis and presentation of results, the qualitative data analysis software Atlas/ti, version 7.1.3 was used. The results pointed to non-linearity in the evolution of U–I interaction and demonstrate that most of the relationships between universities and firms are concentrated in traditional and services channels. Moreover, their interaction intensity is evident in the short term with the flow of knowledge being directed from universities to firms. With regard to benefits and barriers, the research results expand on the avenues outlined in the literature, which reflects some characteristics of this interaction type in Bangladesh, whose relationships are still new and do not yet have a solid trajectory

Keywords: University, Industry, Interaction, Bangladesh



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IICC21-O-10



Transportation, Economics, Energy Options, Environment and Public Health-Need for A Holistic and Sustainable Approach. Case Study of Karachi

Syed Arif Kazmi^{1*}

¹*International Center for Chemical & Biological Sciences, University of Karachi, Pakistan*

**Email: arif.kazmi@gmail.com*

As rural poverty grows, people move towards cities for livelihood. Living spaces become a problem. New neighbourhoods or “Kachi Abadis” which are without essential services spring up all around the city are often far from places of work, a major transportation problem emerges. In the absence of a public transport system ad hoc and individual solutions are sought. With that comes a traffic nightmare. Nearly all vehicles in Karachi use fossil fuels. The air pollution caused by them adversely affects the health of the people who must endure the poisonous environment. An unacceptable number of human hours are wasted getting around the city. Drivers particularly those who must commit a lot of their resources for paying lease instalments and bear the operating expenses for their vehicles have to adjust their family budgets. All this keeps them under a constant stress- a condition which contributes to conditions like diabetes, high blood pressure, heart disease etc. The bad economics of not having a decent transportation, squandering huge funds for facilitating individual transportation using vehicles with polluting internal combustion engines is a tremendous drain on public resources which could be used for betterment of the people. The proposed paper would seek to start a public discourse about solutions of these issues.

Keywords: Fossil Fuel, Energy, Environment, Vehicles.



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IICC21-O-11



Analytical Chemistry: A Gateway to the Sustainable Industry

Huma Shaikh^{1*}

¹National Center of Excellence in Analytical Chemistry, University of Sindh,
Jamshoro, Pakistan

*E-mail:huma.hashu@gmail.com

Composition or more specifically chemical composition of infinite range of materials and products which we use in our professional and personal lives has become a major concern of common man because the quality and quantity of our everyday life performance, the efficiency of our technological equipment, our health and wellbeing all depend on these industrial materials. This concern of common user has put great pressure on the industry to provide all information of composition of its products and to ensure that these products do not contain forbidden or harmful materials or do contain required materials in appropriate quantity. Therefore, an infallible control of every production process is the utmost requirement of Industry and Analytical Chemistry is the universal tool to achieve it. The manufacturing industry is at the verge of expanding its analytical chemistry laboratories in order to keep pace with regulatory requirements, customer demand for data and to produce quality products. Modern Analytical Chemistry is an indispensable instrument in the raw material processing industry because it allows manufacturer to trace the quality of its goods during all manufacturing stages. Precisely, analytical chemistry provides quality assurance to the industrial goods by controlling quality and plays an imperative role in producing sustainable industry.

Keywords: Analytical Chemistry, Industry, Quality Control, Modern Analytical Methods.





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IICC21-O-12



Sustainable Eco-Friendly Fibers in Textile Industry

Syed Muhammad Imtiazuddin^{1*}

¹*Technical Director (Textile), AVM Chemicals Industries, Karachi, Pakistan*

**Email: simtiazuddin@yahoo.com*

The textile industry is considered as the most ecologically harmful industry in the world. The eco-problems in textile industry occur during some production processes and are carried forward right to the finished product. In the production process like bleaching and then dyeing, the subsequent fabric makes a toxin that swells into our ecosystem. During the production process controlling pollution is as vital as making a product free from the toxic effect. The utilization of rayon for clothing has added to the fast depleting forests. Petroleum-based products are harmful to the environment. In order to safeguard our environment from these effects, an integrated pollution control approach is needed. Luckily there is an availability of more substitutes.

Keywords: Textile, Pollution, Rayon, Toxic.



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IICC21-O-13



Development and evaluation of herbal formulations against Acne producing microbes

**M. Hashim Zuberi¹, Abdullah¹, Urooj Haroon^{2*},
Sana Nazeer², Sana Waheed², Sajid Jahangir²**

¹*Department of Environmental Sciences, SMI University, Karachi*

²*Department of Chemistry, Federal Urdu University for Arts, Science &
Technology*

**Email address: uroojharoon@fuuast.edu.pk*

Caring for our skin is one of the easiest ways to ensure long term skin health and radiance. Natural cosmetics development is a progressive startup to provide you with a balance in the skincare and body products you use daily. Unfortunately, many personal care products on the market today, even natural skincare lines, contain hormone-disrupting xenoestrogens. Our main goal is to merge the idea of natural organic skincare products with pharmaceutical standards using nature's own pure ingredients. Organic skincare products are great fun to make as they combine essential vitamins, botanicals, and minerals that heal and restore our skin without harming earth. The development of natural skin care brands are dedicated to redefining beauty industry standards for products that are not only good for us but also good for our planet. At present, we have developed organic soap using different oil blends and herbs. Our organic natural soap recipes are meticulously developed to produce a mild skin nourishing soap that offers a magnificent long lasting lather and leaves your skin feeling clean, soft and radiantly healthy.

Key words: Organic skin care, Natural cosmetics, Soaps, Botanicals.



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IICC21-O-14



Bioplastics: A Green Approach in Materials for Green Environment

Nadia Akram^{1*}, Amina Shafi¹

¹*Department of Chemistry, Government College University Faisalabad,
Faisalabad 38000, Pakistan*

**E-mail: nadiaakram@gcuf.edu.pk*

The diverse and ubiquitous consumption of polymers urges the necessity to make these materials easily available. However, the excessively used petrochemical-based polymers such as Polyvinyl Chloride (PVC) are non-biodegradable, which is a motivation to modify it with “green” alternatives. In the present study, PVC ($MW = 48\,000\text{ g mol}^{-1}$) has been incorporated with cornstarch (CS) to synthesize a series of 25 samples of bioplastics in addition to blank polymer samples. The films of five various thicknesses (0.1, 0.2, 0.3, 0.5, and 1.0 mm) have been synthesized using in situ polymerization. Each sample of pure PVC film and bioplastic has been induced with different concentrations of CS in the range of 1–5 wt %. The synthesized samples were subjected to the structural characterization by using Fourier transform infrared. Thermogravimetric analysis (TGA) has demonstrated the three-step degradation with the improved stability of 250 °C. The 3% concentration of CS has shown the optimum storage modulus (E') of 1.660 MPa from dynamic mechanical analysis (DMA) and the value of $\tan \delta$ as 0.50. The swelling test performed using water has shown an induction of hydrophilicity in PVC up to 4%. CS-induced bioplastics can be a potential ecofriendly alternative of conventional polymers.

Keywords: Green Environment, Bioplastics, Poly Vinyl Chloride, Biowastes, TGA, DMA.



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IICC21-O-15



Need and Impact of Active Pharmaceutical Ingredient Manufacturing on Economic Development and Healthcare System of Pakistan

Tabassum Nusrat¹, Fareeha Lodhi¹, Kounain Farheen¹, Hadiqa Anwar¹, Nusrat Ghani¹, Salman Zafar¹, Muhammad Ali Versiani^{1*}, Sajid Jahangir^{1*}, Kehkashan Khan^{1*}

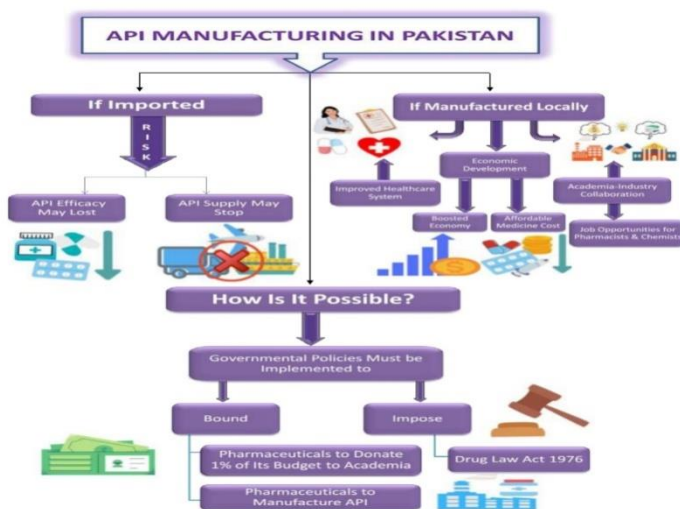
¹Department of Chemistry, Federal Urdu University of Arts, Science and Technology, Karachi, Pakistan

**E-mail: mali.versiani@fuuast.edu.pk, sajid.jahangir@fuuast.edu.pk, kehkashan.khan@fuuast.edu.pk*

Pakistan is a developing country with dynamic pharmaceutical sector. The registered pharmaceutical companies (~650) in Pakistan import 50% active pharmaceutical ingredient (API) from India. Furthermore, out of 820 chemicals utilized in API manufacturing, 62 are imported from India. However, bilateral trade conflicts between the two countries, affects API import and these may lose efficacy during transportation too. Accordingly, in-house API synthesis is essential to maintain its efficacy, reduce cost and burden on economy, which will improve healthcare system of Pakistan. However, a few Pakistani pharmaceutical industries (PPIs) are also synthesizing APIs including cefixime, paracetamol, ibuprofens etc. As per IMS data 2020, PPI market value is of ~453 billion rupees. Moreover, 459MT/year Diclofenac Sodium Inj. is one of the top most imported API, as listed by the Institute of Research Promotion (IRP). Hence, economy of Pakistan may be lifted by manufacturing major imported API. In this context, Government of Pakistan must bound pharmaceuticals to invest at least 1% of its budget for academia to conduct research and development to make API industry self-reliant. In addition to these, practicing drug law act 1976 may also impart positive effect on economy and quality of medicine. Lastly, functional pharmacovigilance must also be implemented.

Keywords: API Import, Efficacy, Boosted Economy, Pharmacovigilance, Governmental Policies.

GRAPHICAL ABSTRACT



Highlights:

- To improve healthcare system by distributing pharmaceutical products of indisputable quality
- To develop link between academia and industry for sustainable lasting future
- To achieve optimum business growth through strong economy for the benefit of all stakeholders



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IICC21-O-16



Synthesis of *Salvia plebia* Silver nanoparticles and Their Dyes Degradation Activity

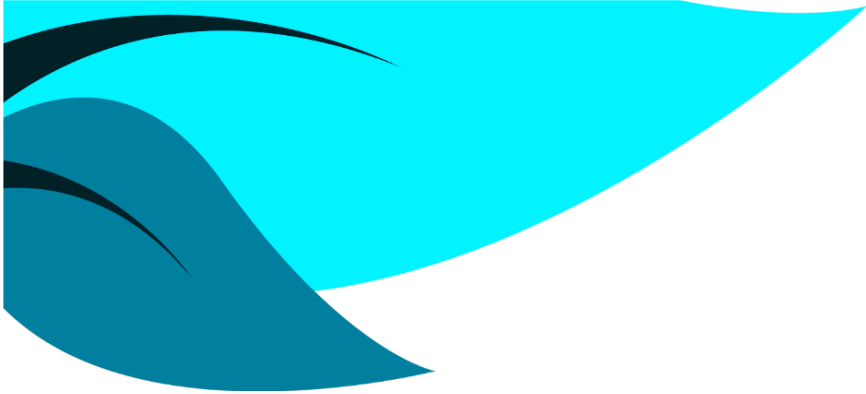
Sana Ihsan¹, Hafiza Salma Bibi¹, Nargis Jamila^{1*}

¹Department of Chemistry, Shaheed Benazir Bhutto Women University,
Peshawar 25000, Khyber Pakhtunkhwa, Pakistan

*Email: nargisjamila@sbbwu.edu.pk

Salvia plebia belonging to family Lamiaceae, is an annual herb widely distributed in Pakistan, China and India. In folk medicine, it has been used to treat hepatitis, inflammation, and cough. Phytochemically, it is a rich source of flavonoids, lignans, and terpenoids specially diterpenoids. In this study, silver nanoparticles (SPAgNPs) are synthesized using *S. plebia* aqueous extract under different conditions of sunlight, stirring, heating and stirring, and incubation in different ratios (1:5 to 1:15). The synthesized SPAgNPs were subjected to determine their catalytic activity in dyes degradation. In synthesis, it was found that 1:9 under heating and stirring afforded significant amount of well stable SPAgNPs as revealed by their sharp UV absorption bands. The synthesized AgNPs also showed very good catalytic activity in the degradation of methyl orange, methylene blue, congo red, *ortho*-nitrophenol and *para*-nitrophenol, which suggests its application in environmental organic pollutant control.

Keywords: *Salvia plebia*, Silver nanoparticles, *o*-nitrophenol, *p*-nitrophenol Dyes.



Technical Session 03

Nanomaterials for Environment



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IICC21-O-18	Photocatalytic Abatement of Congo Red and Methylene Blue in Water using Novel NiO-ZnO-MgO Nanocomposites <u>Naseem Abbas</u> , Nida Rubab, Muhammad Madni, Zeeshan Akhtar, Suryia Manzoor,
IICC21-O-19	Green Synthesis of Recyclable Magnetic Zinc Nanoparticles for The Cost Effective Statistically Optimized Rapid Decontamination of Organic Pollutant from Wastewater <u>Muhammad Saad</u> , Hajira Tahir, Shaista Mehboob
IICC21-O-20	Sulfur and Nitrogen Co-doped Nanoporous Carbon as Sustainable Peroxymonosulfate Activator for Organics Removal <u>Wen-Da Oh</u> , Julia Raudlatul Jannah Zaeni
IICC21-O-21	ZnO QDs/Meso-TiO₂ immobilized on LLDPE film: A Potential Photocatalyst for the Removal of Tetracycline Under Fluorescent Light Irradiation (Graphical Abstract) <u>Anwar Iqbal</u> , Usman Saidu, Farook Adam, Srimala Sreekantan, Noor Fatimah Yahaya, Marzaini Rashid
IICC21-O-22	NanoFormulation of Terminalia Arjuna Bark Extract to Enhance its Therapeutic Potential and Oral Bioavailability <u>Fatiqa Zafar</u> , Nazish Jahan
IICC21-O-23	Magnetic Dispersive Solid Phase Extraction of Traces Cu on Fe₃O₄@XAD-16 <u>Ozgur Ozalp</u> , Mustafa Soylak
IICC21-O-24	Synthesis of Silver Oxalate/Silver Phosphate Nanocomposites for the Cost Effective Statistically Optimized Rapid Decontamination of Organic Pollutant from Wastewater <u>Hafsa Wahid</u> , Mohammad Saad



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IICC21-O-17



Nanotechnology for Safe and Sustainable Environment

Hajira Tahir¹

*¹Department of Chemistry, Faculty of Science, University of Karachi, Karachi,
75270, Pakistan*

**E-mail: hajirat@uok.edu.pk*

Nanotechnology encompasses science, engineering and technology and it involves imaging, measuring, modeling, and manipulating matter at nanoscale. It is big innovation that “The world’s smallest form of technology”. The major Challenges focuses use nanotechnology research: To clean up past environmental damage and correct present environmental problems to prevent future environmental impacts. It helps to sustain the planet for future generations. Recent years have witnessed the devastating impact of climate change on mankind and environment. Nanotechnology is genuinely one such revolutionary field of science with unlimited potential applications. This is evident from some of the greatest breakthroughs in the area of environmental protection, remediation and pollution prevention. With this idea, the present work is set to explore the fundamental aspects and promising applications of nanotechnology with emphasis on its role in environmental sustainability. In short, nanotechnology has significantly contributed to benefiting society and shaping the nature of modern life. It offers opportunities to develop next-generation water supply systems. The extraordinary properties of nanomaterials, such as high surface area, photosensitivity, catalytic and antimicrobial activity, electrochemical, optical, and magnetic properties, and tunable pore size and surface properties, provide useful features for many applications. The development of unique nanoscale structures has the potential to revolutionize industry, including electronics, medicine, and consumer products.

Keywords: Green nanochemistry, Environment conservation, Pollution minimization, Wastewater treatment.



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IICC21-O-18



Photocatalytic Abatement of Congo Red and Methylene Blue in Water using Novel NiO-ZnO-MgO Nanocomposites

Naseem Abbas^{1*}, Nida Rubab², Muhammad Madni¹, Zeeshan Akhtar³, Suryia Manzoor¹,

¹*Institute of Chemical Sciences, Bahauddin Zakariya University, Multan, Pakistan*

²*Department of Physics, Bahauddin Zakariya University, Multan, Pakistan*

³*Department of Applied Chemistry and Chemical Technology, University of Karachi, Pakistan*

**Email: dr.naseem.abbas@bzu.edu.pk*

Water is essential requirement for every living organism in this universe. Most of industrial waste are getting mixed into the river and lakes. Major water pollution caused by textile industries waste which are synthesizing and using dyes to color textile fiber. Mostly Plastic and leather industries are also using dyes for coloring purpose. These dyes get mixed into the water and cannot easily be degraded by traditional methods. These dyes are carcinogenic and may remain in soluble, colloidal or suspended form in water. This study focused on photo degradation of Methylene Blue and Congo Red by NiO-ZnO-MgO metal oxide nanocomposite prepared via co-precipitation and Microwave Assisted Method. Photocatalyst prepared by both methods was characterized by XRD, SEM, EDS and BET. Crystalline structure FCC was confirmed by XRD. By SEM images of sample S2 and S4, particles sizes were found 14 nm and 17nm on average respectively. By EDS presence of Mg, Zn and Ni was confirmed. By BET Surface area 7.726 m²/g, Pore radius Dv(r) 15.979 Å and Pore volume 0.037 cc g⁻¹ was measured. Then composites were applied for degradation of Methylene blue and Congo Red in water solution. Sample with best degradation ability was used for optimization of pH, Catalyst dose, Time change, Effect of Temperature. Results showed that Methylene Blue and Congo red dyes were degraded by prepared composite photocatalyst. Maximum dye degradation obtained, were 86% CR and 90% MB at pH (9.2).

Keywords: Congo red, Methylene Blue, Photo catalyst, Metal Oxide nano composites.



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IICC21-O-19



Green Synthesis of Recyclable Magnetic Zinc Nanoparticles for the Cost Effective Statistically Optimized Rapid Decontamination of Organic Pollutant from Wastewater

Muhammad Saad^{1*}, Hajira Tahir^{1*}, Shaista Mehboob¹

¹Department of Chemistry, Faculty of Science, University of Karachi, Karachi, 75270, Pakistan

*E-mail: saad@uok.edu.pk, hajirat@uok.edu.pk

The current research focuses on the green synthesis of magnetic zinc nanoparticles by *Azadirachta indica* leaves extract. The nanoparticles were characterized by Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray spectroscopy, and Fourier Transformed Infrared Spectroscopy (FTIR). The surface charge was determined by pH_{pzc}. The nanocomposites were employed as high-performance adsorbent for the decontamination of crystal violet dye. The adsorption experiment was optimized by Response Surface Methodology (RSM) based on Central Composite Design (CCD) that predicted a removal of 80.39% under optimum conditions. Replicate 9 runs affirmed the optimum parameters with %RSD and % Mean Error of 1.648% and 2.695% respectively. Significance of model and individual parameters was assessed by ANOVA and pareto analysis. Among various models, Freundlich and pseudo second order models were the best fit isotherm and kinetic models respectively as affirmed by error analyses. Spontaneity of the adsorption process was affirmed by thermodynamic studies. The nanoparticles surface may be regenerated easily in acidic medium and can be used at least for 5 cycles. The adsorption process was studied in presence of several matrices like LiCl, MgCl₂, NaCl, and KCl and it was observed that maximum adsorption took place in presence of low concentration of LiCl salt. Cost analysis indicated a nominal operational cost of US\$ 97.90 m⁻³. Conclusively, the proposed method is an ecofriendly and less expensive method for the environmental remediation purpose.

Keywords: Adsorption, Central Composite Design, Desorption, Nanocomposites, Purification Cost Analysis, Response Surface Methodology, Salt Effect, Wastewater Treatment.



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IICC21-O-20



Sulfur and Nitrogen Co-doped Nanoporous Carbon as Sustainable Peroxymonosulfate Activator for Organics Removal

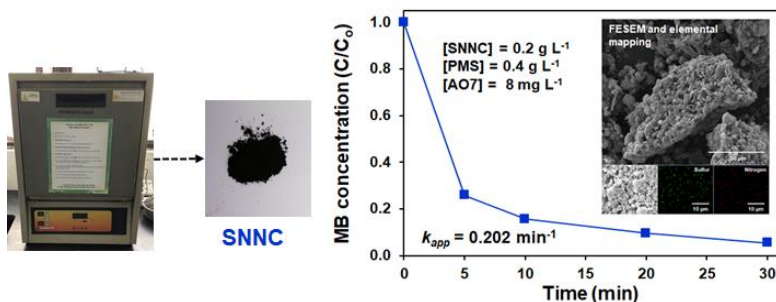
Wen-Da Oh^{1*}, Julia Raudlatul Jannah Zaeni¹

¹School of Chemical Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia

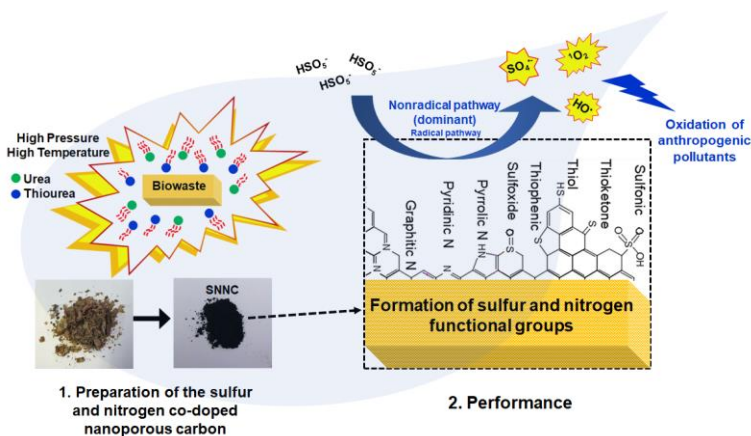
**E-mail: ohwenda@usm.my*

Nanoporous carbon is regarded as an emerging class of carbon allotrope with many important environmental applications. Herein, sulfur and nitrogen co-doped nanoporous carbon (SNNC) was prepared from sawdust via a facile one-pot pyrolysis process. The intrinsic and extrinsic properties of the SNNC was investigated using various characterization techniques indicating that it consists of amorphous carbon phase with porous morphology. The existence of both nitrogen and sulfur functional groups on the carbon surface was also confirmed. The SNNC was employed as peroxymonosulfate (PMS) activator to degrade methylene blue (MB). Notably, SNNC exhibited high MB removal rate with apparent rate constant (k_{app}) = 0.202 min⁻¹. Increasing the SNNC loading and PMS dosage led to positive performance enhancement. The reusability of the SNNC was also studied. While the SNNC performance deteriorated over four cycles, its catalytic activity can be restored using a simple thermal treatment at 500-700°C. The prevailing PMS activation mechanism was investigated using radical scavengers and X-ray photoelectron spectroscopy. The results showed that the nonradical pathway facilitated by the interaction of PMS with graphitic N and thiophenic S was the prevailing pathway. Overall, the results of this study provide a meaningful insight into the application of biowaste as a resource to prepare SNNC for environmental remediation.

Keywords: Nanoporous Carbon, Sulfur and nitrogen Co-doped, Peroxymonosulfate, Waste-to-Resources, Biowaste.



Graphical Abstract:



Highlights:

- S, N Co-doped nanoporous carbon was prepared and characterized.
- Graphitic N and thiophenic S were the active sites for catalysis reaction.
- Performance and mechanism as PMS activator for pollutant removal was studied.



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ZnO QDs/Meso-TiO₂ immobilized on LLDPE film: A Potential Photocatalyst for the Removal of Tetracycline Under Fluorescent Light Irradiation

Anwar Iqbal^{1*}, Usman Saidu^{1*}, Farook Adam¹, Srimala Sreekantan², Noor Fatimah Yahaya³, Marzaini Rashid⁴

¹*School of Chemical Sciences, Universiti Sains Malaysia, Penang, Malaysia*

²*School of Materials & Mineral Resources Engineering, Universiti Sains Malaysia, Engineering Campus, 14300 Nibong Tebal, Seberang Perai Selatan, Pulau Pinang, Malaysia*

³*Integrative Medicine Cluster, Advanced Medical and Dental Institute, Universiti Sains Malaysia, 13200, Kepala Batas, Pulau Pinang, Malaysia.*

⁴*School of Physics, Universiti Sains Malaysia, Penang 11800, Malaysia*

**Email: anwariqbal@usm.my; usmaniyya2000@gmail.com*

The ZnO/TiO₂ nanocomposite powder is known to be an effective photocatalyst for wastewater treatment. However, suspended particles are difficult to be separated for reusability. Hence in this research, ZnO quantum dots /mesoporous TiO₂ (ZnO QDs/meso-TiO₂) nanocomposite was immobilized on linear low-density polyethylene (LLDPE) film for the photooxidation of tetracycline (TC) under fluorescent light (48 watts) irradiation was investigated. The X-ray powder diffraction (XRD) analysis detected the diffraction lines related to anatase TiO₂ and the LLDPE matrix. The thermogravimetric analysis (TGA) indicates that the thermal stability of LLDPE is improved after immobilization with the nanocomposite, and the weight loss for the nanocomposite films was 10%. The diffraction lines related to ZnO quantum dots were not detected due to its low content. The scanning electron microscope (SEM) analysis shows that ZnO quantum dots were deposited inside the pores and on the surface of the TiO₂. The atomic force microscope (AFM) analysis indicates that the surface roughness of the bare LLDPE film increased after immobilization. The water contact angle reduced from 100° for bare LLDPE to 76° for the hybrid film. The reduction in the contact angle suggests the decrease in the crystallinity of the hybrid film and an increase in water absorption. These factors were identified as the main factors in increasing the photocatalytic ability of hybrid film. Within 90 min, 78.9% of TC was removed, whereas no reaction was observed when bare LLDPE was used.

Keywords: ZnO Quantum dots, Tetracycline, Photocatalysis, LLDPE, Photocatalyst.



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Nano-formulation of *Terminalia arjuna* Bark Extract to Enhance its Therapeutic Potential and Oral Bioavailability

Fatima Zafar^{1*}, Nazish Jahan²

¹Department of Chemistry, University of Sahiwal, Sahiwal, Pakistan

²Department of Chemistry, University of Agriculture, Faisalabad, Pakistan

*E-mail: fatiqazafar@uosahiwal.edu.pk

The present study was aimed to enhance the therapeutic potential and oral bioavailability of *Terminalia arjuna* bark extract by using nanosuspension technology. The nanoprecipitation approach being simple and reproducible was successfully used for the preparation of nanosuspension using Polysorbate-80 as a stabilizer. Particle size, polydispersity index, and zeta potential of prepared nanosuspension were measured by using dynamic light scattering technique. DPPH assay was used for determining the antioxidant activity of crude extract and the prepared nanosuspension, whereas, disc diffusion method was used for determining the antimicrobial potential. The in-vitro hemolytic and thrombolytic activities of prepared nanosuspension were determined to evaluate any toxic effect related to nanosuspension. To determine the preeminence of nanosuspension over coarse suspension comparative bioavailability studies were carried out in male albino rats. The formulated nanosuspension of *T. arjuna* showed a mean particle size of 90.53 nm with PDI and zeta potential values of 0.175 and -15.7mV respectively. Comparative evaluation of bioactivities of crude extract and nanosuspension illustrated superior therapeutic potential of *T. arjuna* nanosuspension than coarse extract. The prepared nanosuspension revealed 1.33-fold improved oral bioavailability than its coarse suspension. Overall results showed that nanosuspension technology is an efficient approach to enhance the therapeutic potential and oral bioavailability of *T. arjuna* bark extract.

Keywords: Bioavailability, Nanosuspension, *Terminalia arjuna*, Particle size, Therapeutic potential



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Magnetic Dispersive Solid Phase Extraction of Traces Cu on Fe₃O₄@XAD-16

Ozgur Ozalp^{1,2*}, Mustafa Soylak^{1,2*}

¹Department of Chemistry, Erciyes University, Kayseri, Turkey

²Technology Research and Application Center (TAUM), Erciyes University, Kayseri, Turkey

*E-mail: ozgurozalp@erciyes.edu.tr, soylak@erciyes.edu.tr

Fe₃O₄@XAD-16 has been used as adsorbent for magnetic dispersive solid phase extraction of Cu(II) as with 1-(2-pyridylazo)-2-naphthol (PAN) complex prior to flame atomic absorption spectrometric detection of copper. The effects of important parameters affecting extraction efficiency such as pH, adsorbent amount, eluent concentration and volume, model solution volume, ultrasonic bath time on magnetic solid phase extraction were studied in detail. The optimum pH for the extraction of Cu (II) was 6.0. The enrichment factor was calculated as 25 and the detection limit value (LOD) was found as 10.1 µg L⁻¹. The accuracy of the extraction method was performed by the analysis of HR-1 (river sediment) and TMDA-53.3 (lake water) certified reference materials. The method was applied to determination of copper contents of food, water and other environmental samples.

Keywords: Magnetic solid phase microextraction; Fe₃O₄@XAD-16, Copper; 1-(2-pyridylazo)-2-naphthol (PAN), Flame atomic absorption spectrometry.



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Synthesis of Silver Oxalate/Silver Phosphate Nanocomposites for the Cost Effective Statistically Optimized Rapid Decontamination of Organic Pollutant from Wastewater

Hafsa Wahid^{1*}, Mohammad Saad¹

¹*Department of Chemistry, University of Karachi, Pakistan*

**E-mail: hafsawahid99@gmail.com*

The current research focuses on the synthesis of silver oxalate/silver phosphate nanocomposites by co-precipitation method. The nanocomposites were characterized by Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray spectroscopy and Fourier Transformed Infrared Spectroscopy (FTIR). The surface charge was determined by pH_{pzc}. The nanocomposites were employed as high-performance photo-catalyst for the decontamination of acid red dye. The adsorption experiment was optimized by response surface methodology (RSM) based on central composite design (CCD) that predicted a removal of 96.58% under optimum conditions. Replicate 5 runs affirmed the optimum parameters with %RSD and % mean error of 0.6221% and 1.096% respectively. Significance of model and individual parameters was assessed by ANOVA and pareto analysis. Among various models, pseudo second order model was the best fit kinetic model as affirmed by error analysis. The proposed method is rapid, facile and cost efficient.

Keywords: Photo-catalysis, Central composite Design, Nanocomposites, Purification analysis, Response surface methodology, Wastewater treatment.



Technical Session 04

Recent Catalysts for Environment



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IICC21-O-25	Dye Degradation Screening by Comparative Studies of Catalysis by d-Block Elements <u>Masooda Qadri</u> , Fauzia Muslim
IICC21-O-26	Coal Fly Ash Based Zinc Ferrite Composite as Efficient Photocatalyst for Wastewater Treatment Nimra Nadeem, <u>Muhammad Zahid</u> , Zulfiqar Ahmad Rehan
IICC21-O-27	Synthesis and Characterization of Co-ZnO and Evaluation of its Photocatalytic Activity for Photodegradation of Methyl Orange <u>Muhammad Saeed</u> , Muhammad Adeel
IICC21-O-28	Effect of Surface Roughness on the Efficiency of Hydrogen Evolution Reaction on Gold Surface <u>Faaz Butt</u> , Ramza Siddiqui, M. Sohail Hanif
IICC21-O-29	Simultaneous Catalytic Reduction of Toxic Dyes Using Recyclable Core Shell Nanoparticles <u>Khalida Naseem</u>
IICC21-O-30	Selectivity of Ethylene From Ethanol over Transition Metal Modified Zirconia <u>Nabila Tabassum</u>
IICC21-O-31	Effect of Rod Like Chromium/Manganese Layer Double Hydroxide on Catalytic Degradation of Dyes and Fuel Additive Parameters <u>Sayyed Junaid Ul Hassan Shah</u> , Shanza Rauf Khan
IICC21-O-32	Mesoporous Zn/Co-Ferrites Based High Performance Electrocatalysts for Oxygen Evolution Reaction <u>Kiran Shahzadi</u> , Zahoor Ahmad



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IICC21-O-M-25



Dye Degradation Screening by Comparative Studies of Catalysis by d-Block Elements

Masooda Qadri^{1*}, Fauzia Muslim¹

¹Department of Chemistry University of Karachi-Pakistan

**Email: masoodaq@uok.edu.pk*

In the present studies the phthalocyanine dye was degraded kinetically by “Advance oxidation processes (AOP)”. In the presence of d-block elements the reaction was observed to be dependent on the concentrations of oxidizing agent and phthalocyanine dye. Transition metals helped to facilitate the electron transfer reaction and ultimately involve in the degradation of dye. The reactions were monitored under specific pH range and temperatures to determine the consequences of hydrogen ion concentration on the degradation process. Thermodynamic parameters were also studied to determine the feasibility and nature of reaction by comparing the activities of transition metals. The mechanism of reaction was also elucidated. The present studies show that AOP process is fast and effective process for the removal of dyes and colorants. They can be effectively utilized at industrial scale.

Keywords: Phthalocyanine dye, Hydrogen ion concentration, d-Block, Oxidation



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IICC21-O-26



Coal Fly Ash Based Zinc Ferrite Composite as Efficient Photocatalyst for Wastewater Treatment

Nimra Nadeem¹, Muhammad Zahid^{1*},
Zulfiqar Ahmad Rehan²

¹Department of Chemistry, University of Agriculture, Faisalabad, Pakistan

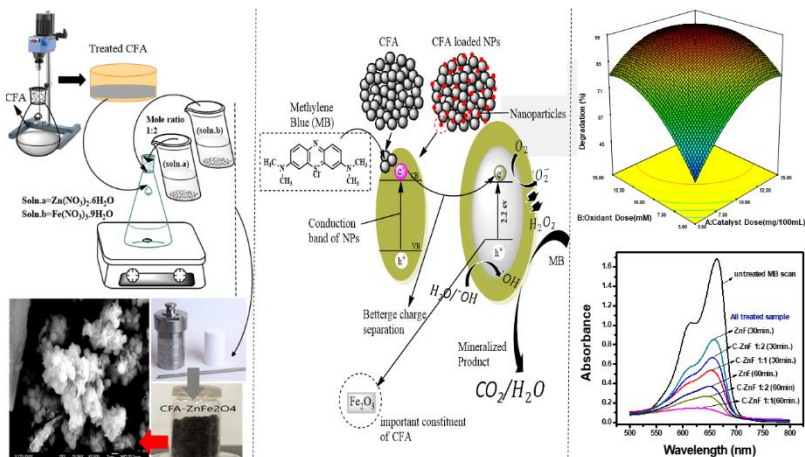
²Department of Polymer Engineering, National Textile University Faisalabad

*E-mail: rmzahid@uaf.edu.pk, zahid595@gmail.com

Three photocatalysts ZnFe_2O_4 , CFA- ZnFe_2O_4 (1:2), and CFA- ZnFe_2O_4 (1:1) were prepared and their comparative dye degradation efficiencies have been evaluated. The catalysts were well characterized using FTIR spectroscopy, XRD, Scanning Electron Microscopy coupled with Energy Dispersive X-ray (SEM-EDX) spectroscopy and Vibrating Sample Magnetometer (VSM). The bandgap energies were calculated using Tauc plot method. The optimization of various parameters like pH, catalysts dose, oxidant dose, reaction time in degradation studies under UV irradiations (254 nm) was done. The optimized conditions of parameters were pH = 3 and 6 for ZnFe_2O_4 and CFA- ZnFe_2O_4 (1:2,1:1) composite, catalysts dose = 8 mg and 10 mg/100 ml for ZnFe_2O_4 and CFA- ZnFe_2O_4 (1:2,1:1) composite, oxidant dose = 14 mM and 10 mM for ZnFe_2O_4 and CFA- ZnFe_2O_4 (1:2,1:1) composite and reaction time = 60 minutes. The ZnFe_2O_4 , CFA- ZnFe_2O_4 (1:2) and CFA- ZnFe_2O_4 (1:1) showed 76, 92, and 97% degradation of MB under optimized conditions, respectively. The photocatalytic degradation results showed that the loading of ZnFe_2O_4 nanoparticles on CFA improves the degradation of MB. The proposed research not only provided a simple approach for the synthesis of CFA based nanocomposites but also reported the reclamation of waste residual material (CFA) to support solid waste management.

Keywords: CFA/ ZnFe_2O_4 , Dye degradation, Photocatalyst, Magnetic composite, Metal ferrite.

GRAPHICAL ABSTRACT:



Highlights:

- Synthesis of coal fly ash (CFA) composites using facile hydrothermal method
- Photocatalytic degradation potential of catalysts was checked under UV light
- Maximum photocatalytic activity was achieved using CFA-ZnFe₂O₄ (1:1)
- CFA-ZnFe₂O₄ showed effective activities up to five time of reusability



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Synthesis and Characterization of Co-ZnO and Evaluation of its Photocatalytic Activity for Photodegradation of Methyl Orange

Muhammad Saeed^{1*}, Muhammad Adeel¹

¹Department of Chemistry, Government College University Faisalabad.

*Email: msaeed@gcuf.edu.pk

Photocatalysis is one of the techniques used for the eradication of organic pollutants from wastewater. In this study, Co-ZnO was tested as a photocatalyst for the degradation of methyl orange under irradiation of visible light. Co-ZnO loaded with 5%, 10%, and 15% Co were prepared by precipitation method. The advanced techniques including X-Ray Diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Diffuse Reflectance UV-visible (DR-UV-Vis) spectroscopy, Photoelectrochemical (PEC) measurements, Temperature Programmed Desorption (TPD), Photoluminescence (PL) and Fluorescence spectroscopy related to OH[•] measurements were used for characterization of prepared Co-ZnO. Experiments showed that 10% Co-ZnO was a highly efficient catalyst for the photodegradation of methyl orange as compared to ZnO. The enhanced photocatalytic activity of Co-ZnO is attributed to the implantation of Co which inhibits the electron-hole recombination. A 100 mg/L solution of methyl orange dye was completely degraded within 130 minutes. The reaction kinetics has been described in terms of the Eley-Rideal mechanism.

Keywords: Co-ZnO, Characterization, Methyl orange, Photodegradation



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Effect of Surface Roughness on the Efficiency of Hydrogen Evolution Reaction on Gold Surface

Faaz Butt^{1*}, Ramza Siddiqui¹, M. Sohail Hanif¹

¹Department of Materials, NED University of Engineering. & Technology,
Karachi, 75270, Pakistan

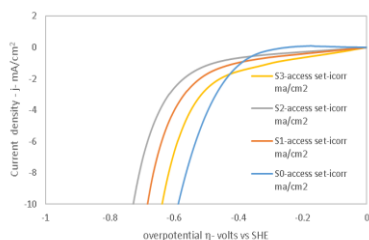
*E-mail:faazbutt@neduet.edu.pk

At present CO₂ in the earth's atmosphere is posing biggest threat to human civilisation. Rising instances of skin diseases, increase in average global temperature, unpredictable weather patterns and melting of polar icecaps along with glaciers can largely be attributed to the presence of CO₂ in the earth's environment. Researchers across the globe are working on developing technologies that can replace C-based fuels for energy. Hydrogen appeared to be the best alternate, that can be coupled with fuel cell systems to meet energy requirements. In the present study, we aim at studying the gold surface for hydrogen evolution reaction. We evaluated gold surface in 1M KCl and found that cold rolled surface has suitable exchange current density of upto $12 \times 10^{-6} \text{ A/cm}^2$ as compare to annealed surface with low value of Tafel slope i.e. 199mV/dec. The samples are tested with XRF, XRD and voltametric studies are carried out using potentiostat.

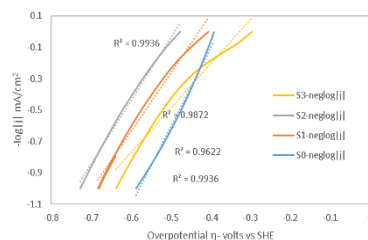
Keywords: Surface roughness, Hydrogen evolution, Hydrogen economy, Catalysis, Electrochemistry



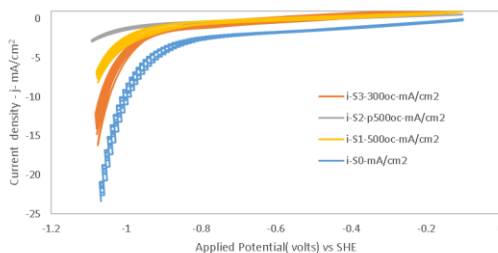
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(a)



(b)



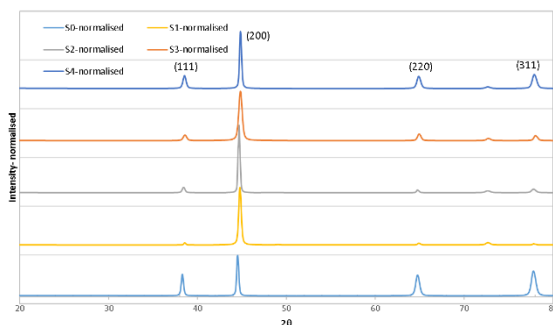
(c)

Electrochemical testing of gold surface for HER in KCL 1M vs SHE against graphite cathode (a) Polarisation curves (b) Plots for exchange current density and Tafel slope (c) Cyclic voltammetry data

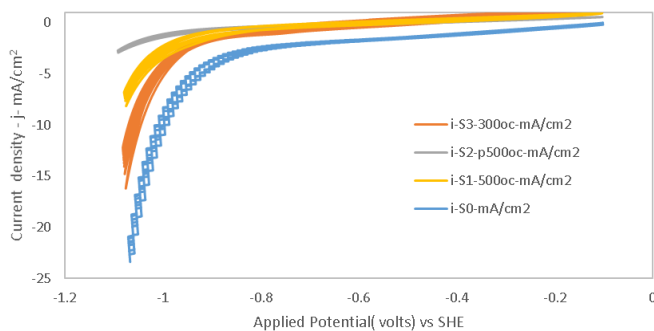
Graphical abstract



HER test setup



XRD patterns for various gold samples



Cyclic voltammetry data for gold surfaces in 1M KCl

Highlights:

- Exchange current densities of up to $10\text{exp}^{-6}\text{A/cm}^2$ with a lowest Tafel slope value of 199mV/dec has been observed.
- Cold rolled samples showed better Tafel slope then annealed and grinded samples.
- Introduction of surface roughness decreases the efficiency of HER on gold surface.



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Simultaneous Catalytic Reduction of Toxic Dyes Using Recyclable Core Shell Nanoparticles

Khalida Naseem^{1*}

¹*Department of Chemistry, University of Central Punjab, Lahore.*

**E-mail: khalidanaseem1@gmail.com*

Industrial effluents consist of various toxic dyes and nitro-aromatic compounds that are harmful to environment and cause large level water pollution. Therefore, removal/degradation of these toxic pollutants from wastewater sources is need of time. Here, silver nanoparticles fabricated polystyrene-poly(N-isopropyl methacrylamide-acrylic acid) core shell particles were prepared via precipitation polymerization method and used as catalyst to degrade toxic dyes such as Congo red (CR), Rhodamine B (RhB) and Methylene blue (Mb) in presence of sodium borohydride (NaBH_4) as reducing agent. Controlled reactions were also performed to prove high activity of core shell nano-catalyst. Pseudo first order kinetic model was applied to investigate the degradation reactions of toxic dyes. It was concluded that prepared composite nano-catalyst increased the rate of reduction reactions and made the reaction kinetically feasible. Nano-catalyst maintained its activity even in case of simultaneous degradation of toxic dyes. Dyes reduction reactions were evaluated on the basis of Langmuir Hinshelwood (L-H) mechanism. Pollutants degradation was also performed under different reaction conditions such as catalyst dose, NaBH_4 and amount of toxic dye. Percentage activity of hybrid catalyst was maintained up to fourth reusability cycle for reduction of toxic dyes.

Keywords: Microgels, Nanoparticles, Dyes, Toxicity, Reduction

Graphical Abstract:

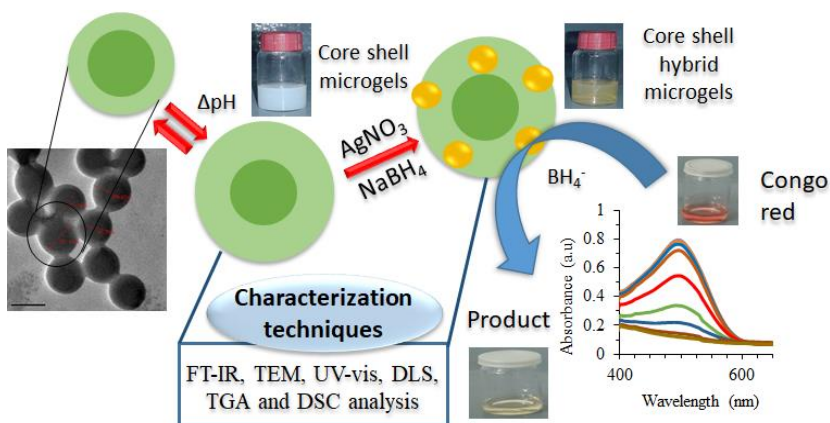


Figure 1. Diagrammatic representation of Ag@PSt-P(NIPMAM-Aac) hybrid particles catalyst for reduction of dye.

Highlights:

- Microgel particles were prepared by precipitation polymerization
- Silver nanoparticles were loaded in shell of core/shell microgel particles
- Hybrid core/shell microgel particles were used for reduction of toxic dyes



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Selectivity of Ethylene from Ethanol over Transition Metal Modified Zirconia

Nabila Tabassum^{1*}

¹*Department of Chemical Engineering, Aliagr Muslim University, UP, India*

**E-mail: tab.naveela84@gmail.com*

Ethanol could be one of the primary sources of hydrocarbons yield used in future transportation. The catalytic conversion of ethanol to olefins attracted many researchers due to the production of petrochemicals and their applications in many industries such as ethylene, polyethylene, polypropylene, etc. The development of a suitable catalyst for the ethanol transformation to olefins can result in several benefits, such as improving conversion, product yield, and lower coke deposition over the catalyst. Metal oxides doped catalysts such as ZrO_2 , and CdO/ZrO_2 were prepared by the co-precipitation method. TGA profiles were recorded to analyze the weight loss during heat treatment to estimate the coke on the catalysts' surface. The X-ray diffraction patterns and Scanning electron micrographs were also taken to investigate the catalysts' surface morphology.

Keywords: Ethylene, Zirconia, Conversion, Selectivity.



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IICC21-O-31



Effect of Rod Like Chromium/Manganese Layer Double Hydroxide on Catalytic Degradation of Dyes and Fuel Additive Parameters

Sayyed Junaid Ul Hassan Shah^{1*}, Shanza Rauf Khan^{1*}

¹Department of Chemistry, University of Agriculture, Faisalabad

*Email: shanza.khan@uaf.edu.pk, junaidshah963@gmail.com

Urea assisted hydrothermal approach is used for synthesis of chromium/manganese layered double hydroxide particles. Manganese accommodate in the LDH lamellar structure. Chromium enhanced the degradation process with adsorption nature of catalyst. The choice of metal combination in this product provides sufficient benefits for this research work. Manganese is proved to be good metal which can accommodate in LDH lamellar structure and enhanced its efficiency. This behavior of lamellae is shown by hydrogen bonds. The parallel alignment, rod-like appearance, surface and dimensions of particles are measured by SEM and STEM. The composition is analyzed by XRD and EDX and formula of LDH is also proposed. Synthesized particles are used as catalyst for degradation of Methyl orange, methylene blue and murexide dyes. Different peaks of characteristics pattern in UV-Vis range are observed. Structures of dyes have different substituent's attached on ring which affect their reactivity. Long conjugated pi-system causes the faster degradation process when catalyst is present in organic compounds. That's why dyes have different behavior in degradation mechanism. kapp of each dye is calculated from results. Effects of catalyst dosages are studied. Flash and fire points, cloud and pour points, kinematics viscosity, specific gravity, surface tension and calorific value of commercial diesel are measured using Cr/Mn LDH.

Keywords: LDH; Nanoneedles, Catalysis, Dye, Degradation.



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Mesoporous Zn/Co-Ferrites Based High Performance Electrocatalysts for Oxygen Evolution Reaction

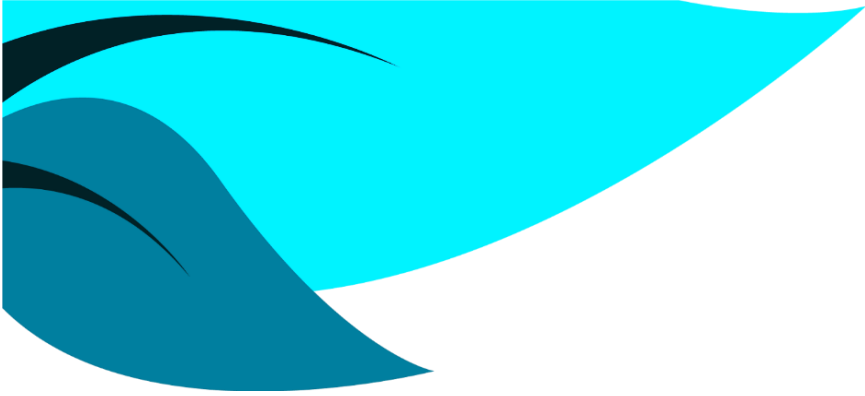
Kiran Shahzadi¹, Zahoor Ahmad^{1*}

¹Department of Chemistry, University of Engineering and Technology Lahore

*Email: zahoorchem@uet.edu.pk

Hydrogen production is more important through water splitting reaction and is of great interest as hydrogen can be used as fuel for automobiles and industries. Herein, hydrothermal synthesis of electrocatalysts viz. $\text{Zn}_{1-x}\text{Co}_x\text{Fe}_2\text{O}_4$ for oxygen evolution reaction in water splitting reaction has been reported. Synthesized electrocatalysts were characterized by various advanced techniques like FTIR, XRD and SEM analyses. The obtained XRD pattern verified the cubic spinel structure of the prepared $\text{Zn}_{1-x}\text{Co}_x\text{Fe}_2\text{O}_4$ electrocatalyst. CV and LSV have been used to check the electrocatalytic activity in terms of onset potential, overpotential and tafel slope of prepared electrocatalyst. EIS studies have also been performed to observe the charge transfer and solution resistance of electrocatalysts. Among the various synthesized electrocatalysts, it has been found that the electrocatalyst with a high content of Co substituted Zn in Zn-ferrites exhibits the highest electrocatalytic activity for OER with low overpotential of 280 mV, low onset potential of 1.51 V, lower charge transfer resistance of 2.1 ohm and a Tafel slope of 65 mV/dec. The electrochemical studies showed that these materials could be potential candidates in water splitting reactions as electrocatalysts for oxygen evolution reaction.

Keywords: Nanoferrites, Electrocatalysis, Oxygen Evolution Reaction



Technical Session 05

Clean Energy & Waste as Valuable Resource



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IICC21-O-33	Utilization of Waste Cooking Oil as Biodiesel Feedstock <u>Mehmood Ali</u> , Muhammad Shahid
IICC21-O-34	Extraction, Purification and Characterization of High-Value Organic Wax from Sugar Industry Bye-Products <u>Saeeda Nadir Ali</u> , Sajid Iqbal, Ali Dad Chandio, Shahid Afghan
IICC21-O-35	Development of Xylanase Based Crosslinked Enzyme Aggregates (CLEAs) and Nanoparticles Based Hybrid System for Paper and Pulp Industries Fehmina Khan, Sumaira Aziz, Asma Ansari, <u>Afsheen Aman</u>
IICC21-O-36	Graphene Based Dye Sensitized Solar Cell <u>Safi Asim Bin Asif</u> , Shaher Bano Asim
IICC21-O-37	Modeling of Hydrate Dissociation Temperature in Pure (CH_4, C_2H_6, C_3H_8) and Mixed Clathrate Hydrate System <u>Khan Muhammad Qureshi</u> , Zubair Chandio, Saima Khan, Sami Chana
IICC21-O-38	Metal Halide Perovskites for Energy Conversion Applications <u>Muhammad Aamir</u>
IICC21-O-39	Comparison of Oven and Solar Drying of Sugarcane Bagasse to Generate Bioenergy <u>Umme Sahar</u> , Mehmood Ali, Mubashir Ali Siddiqui
IICC21-O-40	Biobutanol: A New Biofuel in the Market <u>Syed Wamiq Ali Jafri</u> , Ghulam Mujtaba



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IICC21-O-33



Utilization of Waste Cooking Oil as Biodiesel Feedstock

Mehmood Ali*¹, Muhammad Shahid¹

¹Department of Environmental Engineering, NED University of Engineering and Technology, Karachi-75270, Pakistan

**E-mail: mehmood@neduet.edu.pk*

Due to increase in demand of fossil fuels in the transportation and energy sectors, emissions of combustion product i.e. greenhouse gases are causing climate change and global warming. The importance of alternative sources of energy for CO₂ sequestration is being realized using biofuels to mitigate climate change and global warming. Biodiesel is an alternative fuel to mineral diesel having closed cycle carbon. This research work was based on the production of biodiesel from waste cooking oil (WCO) in a locally designed and fabricated 10L batch scale reactor. WCO was obtained from the NED University canteens and was converted successfully into the biodiesel by two-step esterification and transesterification reactions. In esterification reaction, oil to methanol ratio 5:1 was used, with 0.2% sulphuric acid by weight of oil for reaction time 2 hrs having continuous stirring speed 700 rpm at 65 °C. While in transesterification process, the oil to methanol molar ratio was 5:1 with KOH as catalyst 1% weight of WCO at 65 °C temperature, mixing speed 700 rpm for 1 hr. reaction time. The yield of biodiesel produced from 10L WCO was 9.27 L (92.7% by volume of oil) and glycerine 7.3 L as a by-product of transesterification reaction. The biodiesel produced was characterized and its properties were found in accordance with International Biodiesel Standards ASTM D6751 and EN 14214. Production of biodiesel from WCO in future would help to mitigate climate change, improves energy security and sustainable development in the renewable energy sector in Pakistan.

Keywords: Alternative fuel, Biodiesel, Waste cooking oil (WCO), Transesterification, Climate change



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IICC21-O-34



Extraction, Purification and Characterization of High-Value Organic Wax from Sugar Industry Bye-Products

**Saeeda Nadir Ali^{1*}, Sajid Iqbal², Ali Dad Chandio³,
Shahid Afghan⁴**

¹*Department of Chemistry, NED University of Engineering. & Technology,
Karachi, Pakistan*

²*Department of Chemistry, Jinnah Govt. College for Boys, Nazimabad Karachi,*

³*Department of Metallurgical Engineering, NED University of Engineering. &
Technology, Karachi, Pakistan*

⁴*Sugar Research and Development Board, Government of Punjab, Pakistan.*

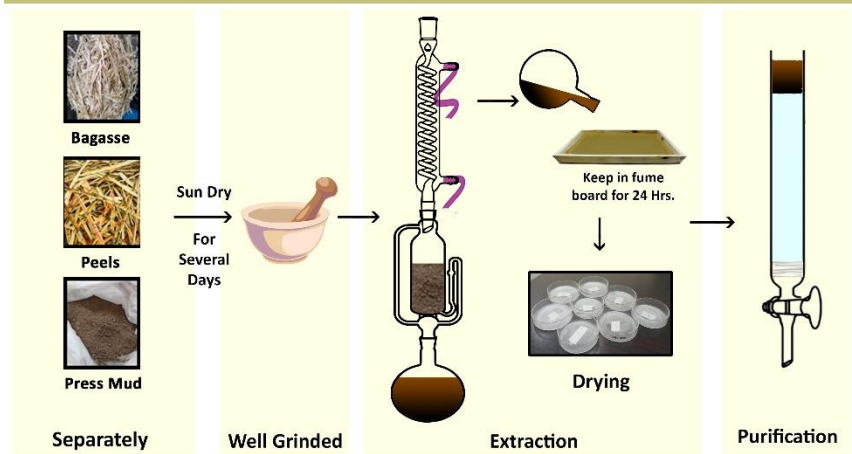
**E-mail: saeeda@neduet.edu.pk*

In the present study, bye-products obtained during sugar manufacturing process were used to extract high-value organic wax for sustainable bioeconomy development. The extraction from sugarcane peels, bagasse and press mud was carried out using soxhlet apparatus by means of hexane as extraction solvent and yield was investigated. UV-Visible spectra of sugarcane wax showed maximum wavelength at 227 nm. The chemical characterization including FT-IR and GC-MS indicates the presence of fatty acids, esters, alcohols and long chain alkanes. In addition, XRD analysis showed intensified peaks at $2\theta=21.39$ and 23.71 indicating the occurrence of the amorphous region. TGA was performed for thermal characterization.

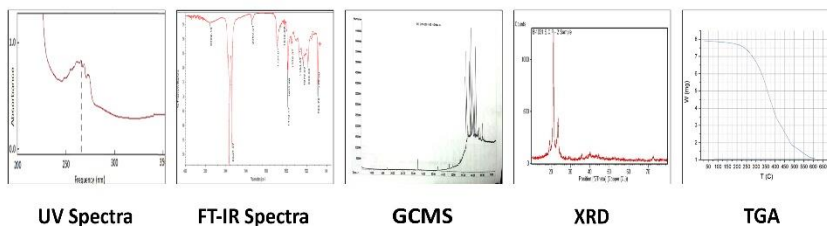
Keywords: Sugar industry bye-products, Peels, Bagasse, Extraction, Hexane, Organic wax

Graphical Abstract:

Extraction & Purification



Characterization



Highlights:

- Extraction of organic wax for sugar cane peels, bagasse and press mud.
- Purification of extracted organic wax.
- Characterization of wax through UV, FT-IR, GCMS, XRD, and TGA techniques.



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IICC21-O-35



Development of Xylanase Based Crosslinked Enzyme Aggregates (CLEAs) and Nanoparticles Based Hybrid System for Paper and Pulp Industries

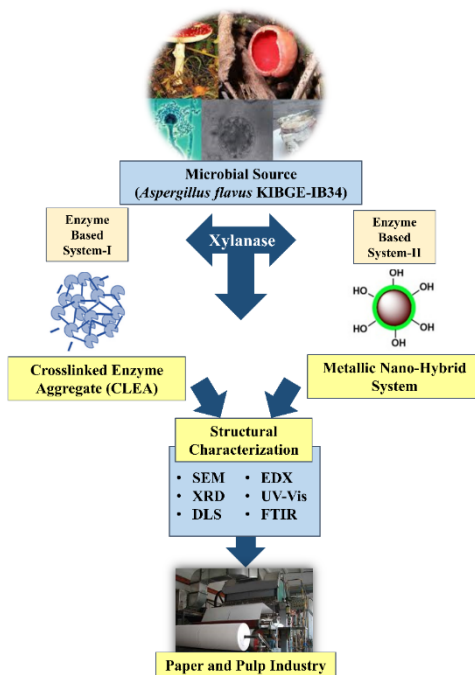
Fehmina Khan¹, Sumaira Aziz¹, Asma Ansari¹,
Afsheen Aman^{1*}

¹*Dr. Abdul Qadir Khan Institute of Biotechnology & Genetic Engineering
(KIBGE), University of Karachi, Karachi, Pakistan*

**E-mail: afaman@uok.edu.pk*

Microbial enzymes are now industrially desirable and have replaced traditional chemical treatments because they catalyze reactions rarely that produces wasteful metabolites. Enzyme based catalysis generally do not pose any environment threat and therefore, helps in achieving sustainable goals during industrial processing. Most recognizable enzyme class used in industrial setups belongs to the family of hydrolases. Paper and pulp, textile and food industries are some of the businesses that utilizes enzymes frequently. Cellulases remains prominent enzyme along with xylanases for the treatment of paper and pulp and also for paper recycling. Current research focuses on utilization of microbial xylanases for the development of two innovative systems that could mediate enzyme catalyzed reactions much faster and are recovered back after effective treatment. First system is development of xylanase based crosslinked enzyme aggregate (CLEAs) while, second system is the fabrication of metallic nano-hybrid system comprising xylanase as a biocatalyst. Both xylanase based structures were characterized using advanced analytical techniques in order to confirm their structural integrity. Both developed systematic units, are easily recoverable using either a filtering system or magnetic field. Thus, becomes plausible candidates for paper and pulp industry by lowering adverse environmental impact that is generally seen during conventional chemical treatments.

Keywords: Crosslinked Enzyme Aggregates, Nano-Hybrid System, Iron Nanoparticles, Xylanase, Paper and Pulp Industry.



Highlights:

- Xylanase based crosslinked enzyme aggregates (CLEA) were developed.
- Xylanase based metallic nano-hybrid system was fabricated.
- Both structures could be used in paper and pulp industry.



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IICC21-O-36



Graphene Based Dye Sensitized Solar Cell

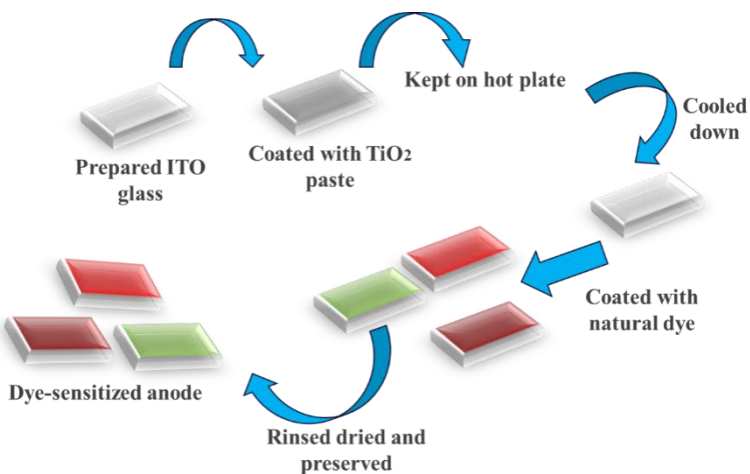
Safi Asim Bin Asif^{1*}, Shaher Bano Asim¹

¹*Analytical Chemistry Section, Department of Chemistry, Faculty of Science,
University of Karachi, Karachi, Pakistan*

**E-mail: safi.asim@uok.edu.pk*

Globally, there is a great need of producing alternative source of electrical energy, especially in Pakistan. Out of various ways of alternative energy, photovoltaic cells (solar cells) are promising devices to overcome the energy crisis. Dye-sensitized solar cells (DSSC) are fascinating the global market owing to its easiest fabrication, cost effectiveness and low toxicity. This research present the remarkable achievement in fabrication of low-cost DSSC. Previously, research has been done to improve durability and efficiency of cells. The dye, usually organic natural or synthetic, adsorbed titanium dioxide (TiO_2) is coated over the surface of substrate (works as cathode) i.e. Indium tin oxide (ITO) glass. In the current research, two different and novel approaches has been made. 1) ITO cathode has been replaced by metal-glass substrate, 2) Anode electrode is fabricated with Graphene based Nanocomposites. The aim of both approaches is to reduce price and improve electrical efficiency of dye-sensitized solar cell. Three natural pigments (Betain, Anthocyanin and Chlorophyll) have been implemented in DSSC as dye-sensitizers. In DSSC, dyes are crucial since these are electrons suppliers after absorbing visible light. These makes DSSC non-toxic, easiest and cost-effective cells. Despite the limitation of natural dyes, the advantages include high absorption coefficients, low cost extraction and low toxicity.

Keywords: Graphene based Nanocomposites, Dye Sensitized Solar Cells, Alternative Energy, Betain, Anthocyanin and Chlorophyll.



Highlights:

- Graphene based nanocomposite has been synthesized.
- Natural dyes has been used for the sensitization.
- Efficiency in light conversion electricity has been observed.



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Modeling of Hydrate Dissociation Temperature in Pure (CH_4 , C_2H_6 , C_3H_8) and Mixed Clathrate Hydrate System

Khan Muhammad Qureshi^{1*}, Zubair Chandio², Saima Khan³, Sami Chana⁴

¹*Chemical Engineering Department Mehran University of Engineering and Technology Jamshoro Sindh, Pakistan.*

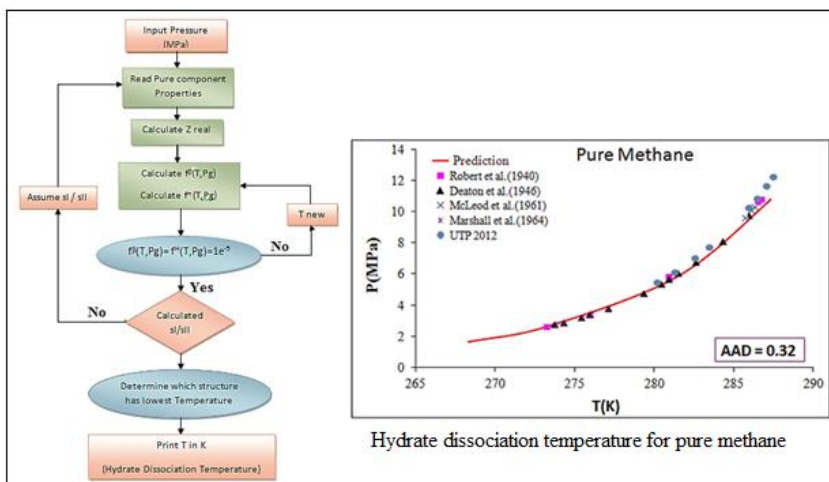
³*Department of Chemical Engineering, University of Malaya 50603, Kuala Lumpur Malaysia.*

^{2,4}*Quaid-e-Awam University of Engineering, Science and Technology, QUEST Nawabshah, Pakistan*

**E-mail: khan.muhammad@faculty.muett.edu.pk*

Model of pure CH_4 , C_2H_6 , C_3H_8 and mixed clathrate hydrate system is developed to predict the hydrate dissociation temperature. Phase diagram is developed which has valuable worth and can be used to provide the phase behavior information in design of distillation column, methane, ethane, carbon dioxide storage and effective recovery in chemical process industry. A mathematical tool (Matlab) is used for single and ternary systems to code SRK Eos. To confirm the different structures, van der Waals and Platteeuw (vdWP) model and Kihara parameters were used to get mutual gas and water solubility. Modelling results showed that hydrate model parameters can fit the data well with the previous model. The viscosity and the second virial coefficient are determined from the published data by the Kihara potential parameters. SRK-Eos is effectively tested in contrast with measured values for pure methane, ethane and propane. Similarly, for multi-component ethane+methane+water system is found with (AAD=0.34). The less value of AAD showed the reliability of this mathematical model. Therefore, modelling results are in agreement with experimental data.

Keywords: Hydrate, Modelling, Dissociation, Ternary System.



Highlights:

- Mixed clathrate hydrate system is developed to predict the hydrate dissociation temperature.
- Matlab is used to code SRK Eos for single and ternary systems prediction.
- Modelling results are in agreement with the experimental data.



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Metal Halide Perovskites for Energy Conversion Applications

Muhammad Aamir^{1*}

¹*Materials Laboratory, Department of Chemistry, Mirpur University of Science and Technology (MUST), Mirpur-10250 (AJK), Pakistan*

**E-mail: aamirorg@gmail.com*

Metal halide perovskites have emerged as an efficient light harvesting material for solar cells and LEDs. We developed metal halide perovskite materials for sensing, photocatalysis and photovoltaic applications. Owing to an efficient emitter, metal halide perovskite has shown good fluorescent sensing of lead ions, water and explosives. Apart from sensing applications, morphology controlled thin films were deposited by aerosol assisted chemical vapour deposition (AACVD). The planar solar device based on CsPbBr₂I bulk perovskite has shown the PCE of 4.8% on the other hand, broad band emission and green emissions were also observed in metal halide perovskites. Interestingly, the compositional manipulations and the OHNH₃PbX₃ hybrid perovskites were successfully used for the degradation of commercial dye.

Keywords: Metal Halide Perovskite, Light Harvesting Materials, Light Emitters, Sensing, Photocatalysis



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Comparison of Oven and Solar Drying of Sugarcane Bagasse to Generate Bioenergy

Umme Sahar¹, Mehmood Ali^{1*}, Mubashir Ali Siddiqui²

¹*Department of Environmental Engineering, NED University of Engineering and Technology, Karachi*

²*Department of Mechanical Engineering, NED University of Engineering and Technology, Karachi*

**E-mail: mehmood@neduet.edu.pk*

High moisture content in agricultural residue causes major hindrance in its utilization for producing bioenergy with lower calorific value (CV). This research study was conducted to compare solar cabinet box dryer and conventional oven to enhance its CV. The CV of raw bagasse was found 9.34 MJ kg^{-1} with 50.8 % moisture content on wet basis. By using solar cabinet box drying, CV was improved to 19.06 MJ kg^{-1} with 5 hrs treatment time and with moisture content removal of 28.10 % on wet basis, while with conventional oven drying it was enhanced to 19.25 MJ kg^{-1} with moisture removal of 31.34%. The bulk density of raw bagasse was found 156.75 kg m^{-3} , while it was reduced to 111.32 kg m^{-3} with solar drying for 5 hrs treatment time and 110.23 kg m^{-3} with oven drying treatment. Particle size distribution showed that the particles retained from sieve size of 0.25 mm from oven treatment method were less i.e. 12.015 g, while the particles retained with solar drying was higher in quantity 12.989 g after 5 hrs. The statistical analysis (ANOVA) showed that the *p-value* of oven dried sample was 0.0001 and for the solar drying treatment was 0.0067 at 95 % confidence interval. The statistical result observed that oven drying creating more significant influence in terms of moisture content removal as compared to solar drying. It is recommended to use agricultural residues such as bagasse with enhanced calorific value as a promising feedstock to produce bioenergy in Pakistan.

Keywords: Bagasse, Calorific Value, Solar Drying, Moisture content, ANOVA.



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IICC21-O-40



Biobutanol: A New Biofuel in the Market

Syed Wamiq Ali Jafri^{1*}, Ghulam Mujtaba²

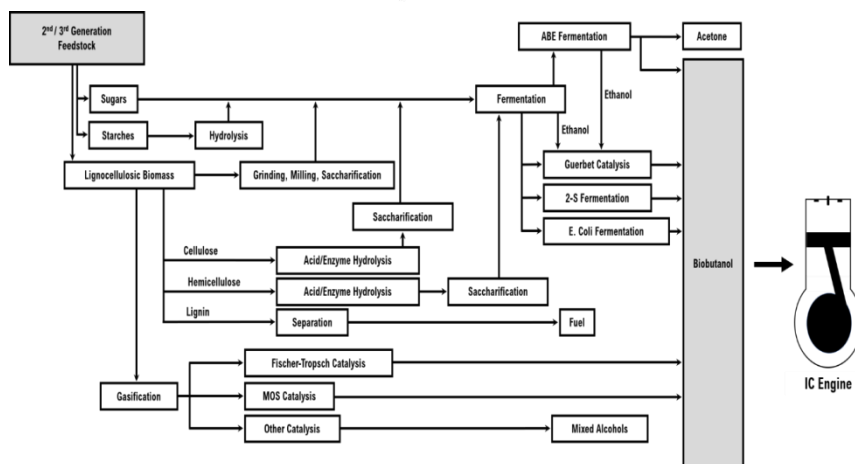
¹*Department of Mechanical Engineering, NED University of Engineering & Technology, Karachi, 75270, Pakistan*

²*Department of Energy & Environment Engineering, Dawood University of Engineering & Technology, Karachi, 74800, Pakistan*

**E-mail: wamiq.ali90@gmail.com*

Biobutanol is a biofuel which comes from biological origin and is an attractive biofuel because of its properties such as energy density and octane rating etc. It is a sustainable renewable fuel to use in transportation sector then other biofuels like bioethanol and biomethanol because of its great resemblance with gasoline (and diesel). Even it is also a good blending and replacement option for conventional internal combustion engines, the purpose is one to use and promote a clean energy source because of environmental consensus and global climate change issues. Current study is focus on the biobutanol, its characteristics, its production routes from sustainable processes with low production rate and high yield, and also to promote this feasible biofuel. The focus is on 2nd and 3rd generation biofuels to consume waste and utilize them for bioenergy.

Keywords: Renewable Energy, Sustainable Biofuel, Biobutanol, 2nd and 3rd Generation Feedstock, Transportation Sector.



Highlights:

- Biobutanol is one of a promising biofuel
- Properties of Biobutanol are very much resemble with gasoline showing that it is a better blending and replacement option
- It can be produce through several routes by using 2nd and 3rd generation feedstocks.



Technical Session 06

Chemistry for Industrial Sustainability-II



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IICC21-O-41	Adsorption Research from Pakistan in Last 30 Years: Scientometric Assessment of Trends and Developments <u>Amtul Qayoom</u> , Ming-Huang Wang, Saeeda Nadir Ali, Yuh-Shan Ho
IICC21-O-42	Modification and Characterization of Silica Extracted from Rice Husk for Adsorptive Removal of Methyl Orange from Aqueous Media <u>Syed Shafqat</u> , Nouman Hamid
IICC21-O-43	Removal of Halosulfuron Methyl Herbicide from Aqueous Media Using Neem Seeds: Kinetic, Equilibrium and Thermodynamic Studies <u>Atta ul Haq</u> , Muhammad Kashif
IICC21-O-44	Designing and Characterization of Ion Exchange Membranes. <u>Shazia Perveen</u> , Ruba Khawar, Muhammad Taha Bin Siraj
IICC21-O-45	Effect of Inhibitors on Corrosion Rate of UEP Pipelines in Different Oil and Brine Mediums Abdul Rauf Jamali, Ali Dad Chandio, Iftikhar Ahmed Channa, <u>Jahanzeb Bhatti</u>
IICC21-O-46	Polystyrene Degradation into Value-Added Products over Copper Based Catalyst and Their Recycling in Bulk <u>Adnan</u> , Jasmin Shah, Muhammad Rasul Jan
IICC21-O-47	Phytoremediation of Heavy Metal Contaminated Soil Using Four Non-Hyperaccumulator Plants Species: A study on Green Technology Hira Amin, Basir Ahmed Arain, Taj Muhammad Jahangir, Abdul Rasool Abbasi, Muhammad Sadiq Abbasi, <u>Farah Amin</u>
IICC21-O-48	Chemical Oxygen Demand (COD) Reduction in Petrochemical Wastewater by Ozonation Method <u>Muhammad Ammar</u> , Syed Farhan Hasany, Syed Ghazanfar Hussain



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IICC21-O-41



Adsorption Research from Pakistan in Last 30 Years: Scientometric Assessment of Trends and Developments

**Amtul Qayoom^{1*}, Ming-Huang Wang², Saeeda Nadir Ali¹,
Yuh-Shan Ho³**

*¹Department of Chemistry, NED University of Engineering and Technology,
Karachi, Pakistan*

*²Department of Environmental Sciences and Engineering, Inner Mongolia
University of Technology, China*

*³Trend Research Centre, Asia University, No. 500, Lioufeng Road, Wufeng,
Taichung County 41354, Taiwan*

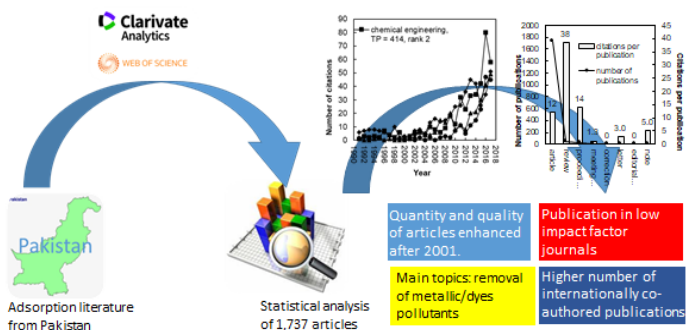
**Email: amtulq@neduet.edu.pk*

In present work, scientometric tools were used to assess trends and quality of adsorption related research contribution from Pakistan. For this purpose, adsorption related research contribution by Pakistani researchers from 1991 to 2017 have been analyzed. Statistical analysis of selected publications was conducted on the basis of total number of citations since publication to the end of the recent year, the number of citation of an article in recent year only, the total number of citations for an article in its publication year, and the total number of citations per year. A sharp increase in research output was observed after year 2000 which may be credited to reform of Higher Education Commission in Pakistan. Almost 95% adsorption related articles from Pakistan have been published low impact factor journals. Multidisciplinary chemistry journals published most of adsorption related Pakistani articles with maximum publications in Journal of the Chemical Society of Pakistan. Among various research institutes, University of Peshawar, Pakistan ranked first on the basis of total number of articles, first author articles, and corresponding author articles. Six most highly cited publications belonged to Pakistan Council of Scientific and Industrial Research (PCSIR). Number of international collaborative publications increased since 1991 to 2017 and resulted in their ratio being higher as compared to single institutional or nationally collaborative publications. The main focus of adsorption related literature from Pakistan since 1991 to 2017 was removal of metallic or dye contaminants from water and/or industrial effluents.

Keywords: Adsorption, Scientometric, Pakistan, SCI-EXPANDED, Y-index



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Highlights:

- Quantity and quality of Pakistan adsorption related articles enhanced after 2001.
- Most of the adsorption related articles from Pakistan published in low impact factor journals
- Number of internationally co-authored publications is higher as compared to single institution and nationally co-authored publications
- Main focus of Pakistan adsorption related publication remained removal of metallic and dyes pollutants from aqueous solutions.



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IICC21-O-42



Modification and Characterization of Silica Extracted from Rice Husk for Adsorptive Removal of Methyl Orange from Aqueous Media

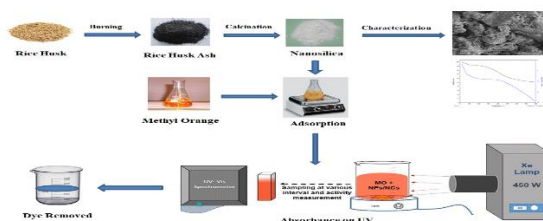
Syed Shafqat^{1*}, Nouman Hamid¹,

¹Department of Chemistry, Division of Science & Technology, University of Education, Lahore, Pakistan

*E-mail: salman.shafqat2ue.edu.pk

Due to the color, sensitivity, oxidative metabolism and cytotoxicity of the dyes, the release of azo dyes into the atmosphere is at high risk for living organisms. In the present study, the removal of methyl orange an azo dye from waste water was conducted by unmodified and modified amorphous nanosilica extracted from agro-waste rice husk ash. Efficient removal of methyl orange was observed by using magnetically activated rice husk silica (A-RHS) as compared to unmodified silica (RHS). Modification of bisorbent was confirmed by characterization through FTIR, SEM, TGA and DSC. Batch bisorption was performed using well established adsorption parameters including adsorbent dose, contact time and pH of medium. Optimum condition for the highest %age removal (82% for RHS, 85% for A-RHS) was found to be 0.3g at 25 minutes for RHS and 20 minutes for A-RHS at pH 3.1. The experimental data obtained verified that Langmuir model was found to be best fitted with this study (R^2 was 0.9953 for RHS and 0.9946 for A-RHS) and follows pseudo 2nd order model during bisorption ($R^2 = 0.9986$ for RHS and 0.9998 for A-RHS).

Keywords: Nanosilica, Modified, Methyl Orange, Rice Husk.





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IICC21-O-M-43



Removal of Halosulfuron Methyl Herbicide from Aqueous Media Using Neem Seeds: Kinetic, Equilibrium and Thermodynamic Studies

Atta ul Haq^{1*}, Muhammad Kashif¹

¹Government College University Faisalabad, Pakistan

*Email: attaulhaq@gcuf.edu.pk

In the present study, the removal of Halosulfuron methyl from aqueous solution was carried out using neem seed powder (NSP). The removal study was conducted in batch system under the effect of several operational parameters such as pH, sorbent dose, contact time, initial Halosulfuron methyl concentration, agitation time and temperature. Surface area analyzer (SAA), Energy Dispersive X-ray (EDX), and Scanning electron microscopy (SEM) tests were performed before and after the sorption process. The maximum removal was achieved at pH 3. The removal data of the Halosulfuron methyl was fitted to the various kinetic models and the result showed that kinetic data well fitted into intraparticle diffusion kinetic model not only due to high value of R^2 (0.92). Sorption data was also fitted into various isotherms and the result showed Langmuir isotherm is the best one to explain the data due to its high R^2 value (0.92). Thermodynamic parameter such as enthalpy, free energy and entropy were also calculated and showed that removal of Halosulfuron methyl using neem seeds is exothermic and spontaneous process.

Keywords: Halosulfuron Methyl, Biosorption, Kinetic, Equilibrium, Thermodynamic.



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IICC21-O-44



Designing and Characterization of Ion Exchange Membranes

Shazia Perveen^{1*}, Ruba Khawar¹, Muhammad Taha Bin Siraj¹

¹*Department of Chemistry, NED University of Engineering and Technology,
Karachi, Pakistan*

**Email: shaziaperveen@neduet.edu.pk*

With energy cost rising and environmental problems worsening, the challenge currently lies in the production or storage of energy and supply of fresh water by renewable and sustainable resources. Ion exchange membranes (IEMs) have attracted much attention to achieve the energy task and to alleviate environment related issues. Ion exchange membranes have wide-ranging applications from pharmaceuticals to waste treatment, desalination to water purification and energy production to energy storage. Ion exchange membranes (IEMs) are characterized as key component of the electrochemical cell to achieve the energy task. Redox flow batteries and Reverse electrodialysis (RED) are the most promising technologies for energy storage and energy conversion respectively. Due to significant applications of ion exchange membranes, there is a great need to design low cost membranes and hence this work has been planned. Present study will establish synthetic methods for designing and characterization of IEMs. This study is a comprehensive overview of the designing of ion exchange membrane and their application leading to the synthesis of anion exchange membrane. Synthesized membranes have been characterized and morphology was studied through SEM, AFM and compounds were confirmed through IR.

Keywords: Ion exchange membranes, Renewable energy resources, Sustainable development goals, Redox flow batteries, Reverse electrodialysis.



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IICC21-O-45



Effect of Inhibitors on Corrosion Rate of UEP Pipelines in Different Oil and Brine Mediums

Abdul Rauf Jamali^{1*}, Ali Dad Chandio², Iftikhar Ahmed Channa², Jahanzeb Bhatti²

¹Department of Materials Engineering, NED University of Engineering. & Technology, Karachi, Pakistan

²Department of Metallurgical Engineering, NED University of Engineering. & Technology, Karachi, Pakistan

*Email: engrabdulrauf@neduet.edu.pk

From several years, crude and refined oil have been playing an important role in economic development. Hence, efforts have been made to properly maintain the transportation of such oil with minimal losses. Corrosion is one of the greatest issue that may harshly reduce service life of pipelines. This can be prevented by plenty of techniques (i.e. inhibitors). Different inhibitors were used namely EC-1392 (for oil) and EC-1304 (for water). In present work, oil pipelines used in different fields of UEP (United Energy Pakistan) that carry crude oil was obtained. Effect of corrosive mediums on the oil pipeline was examined by using weight loss method. Samples of the oil pipeline were kept dipped in these acidic mediums for a period of time ranging from 1-40days, inspection was carried out with a gap of 10days. Potentiostat tests and SEM inspection were also carried out to determine effects of inhibitor and rate of corrosion. It found that by selecting the right quantity of inhibitor injection with respect to the medium and time duration will cause reduction in metal losses and also that in these mediums the metal (X-52 SS) should never be used without inhibitor film or else the losses can be catastrophic.

Keywords: Inhibitor, Corrosion, Crude Oil, Potentiostat, Pipeline.



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IICC21-O-46



Polystyrene Degradation into Value-Added Products over Copper Based Catalyst and their Recycling in Bulk

Adnan^{1,2*}, Jasmin Shah², Muhammad Rasul Jan²

¹*Institute of Chemical Sciences, University of Swat, KPK, Pakistan.*

²*Institute of Chemical Sciences, University of Peshawar, KPK, Pakistan.*

**Email: adnanchem@uswat.edu.pk*

Catalytic degradation of WEPS was carried out using Cu metal, CuO and CuCl₂ as catalysts. Catalytic degradation of WEPS was found to produce selective products i.e. low molecular weight aromatic hydrocarbons with minimum amount of residue, gases and unwanted high molecular weight aromatic hydrocarbons. Cu and Cu containing catalyst decreased the activation energy with high activity. Maximum yield of liquid products were 93.93 wt.% with 450 °C, 30 min reaction time and 1:0.3 polymer to catalyst ratio, maximum liquid products were 90.27 wt.% and 91.40 wt.% with CuO and CuCl₂ catalyst with 450 °C, 30 min reaction time and 1:0.2 polymer to catalyst ratio. Cu metal was found the best catalyst among the used catalysts with liquid products yield of 93.93 wt.%, styrene selectivity of 55.14 wt.% and styrene monomer recovery of 60 wt.%.

Keywords: Polystyrene (PS), Catalyst, Degradation, Fractional distillation, Degradation in bulk.



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Phytoremediation of Heavy Metal Contaminated Soil Using Four Non-Hyperaccumulator Plants Species: A Study on Green Technology

Hira Amin¹, Basir Ahmed Arain¹, Taj Muhammad Jahangir²,
Abdul Rasool Abbasi³, Muhammad Sadiq Abbasi⁴,
Farah Amin^{5*}

¹Institute of Plant Sciences, University of Sindh, Jamshoro, Pakistan

²Institute of Advanced Research Studies in Chemical Sciences, University of Sindh

³Department of Fresh Water Biology and Fisheries, University of Sindh

⁴Department of Mathematics & Statistics, Quaid-e-Awam University of Engineering,
Science & Technology, Nawabshah, Pakistan

⁵National Centre of Excellence in Analytical Chemistry, University of Sindh

*Email: farahamin00@gmail.com

Soil contamination by heavy metals is a serious issue faced by several countries around the world, and conventional technologies to resolve this problem were expensive and caused negative impact on the environment. One solution to reduce the concentrations of heavy metals in soil is to use plants that can absorb and accumulate heavy metals into harvestable parts, a process referred as phytoremediation. To understand the plant's potential, a pot experiment was conducted with four non-hyperaccumulator plants species i.e., *Abelmoschus esculentus*, *Avena sativa*, *Cyamopsis tetragonoloba* and *Sesamum indicum*. The selected plants were allowed to grow in metal contaminated soil for 12 weeks. At the end of experimental period, plants were harvested and then analyzed for metal tolerance and extraction. Among the four non-hyperaccumulator plants investigated, the germination and growth parameters along with chlorophyll contents were significantly ($p < 0.05$) higher in *A. sativa* followed by *C. tetragonoloba*, *S. indicum* and *A. esculentus*. Likewise, *A. sativa* exhibited highest bioconcentration factor (1.34 and 1.30), bioaccumulation coefficient (1.71 and 1.50), translocation factor (1.28 and 1.16) and phytoremediation efficiency (4.81% and 5.17%) for Cu and Zn, respectively suggested that *A. sativa* was suitable for phytoextraction. On the other hand for Pb, the values of BCF (1.62), BAC (0.89), TF (0.55) and PR (21.74%) suggested that *A. sativa* has the great capacity to tolerate and stabilized high concentrations of Pb than other tested plants. From the experimental results, it was concluded that being non-hyperaccumulator, *A. sativa* has ability to remediate metal contaminated soil effectively up to allowable limits.

Keywords: Soil pollution, Heavy metals, Tolerance, Accumulation, Phytoremediation.



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IICC21-O-M-48



Chemical Oxygen Demand (COD) Reduction in Petrochemical Wastewater by Ozonation Method

**Muhammad Ammar^{1*}, Syed Farhan Hasany²,
Syed Ghazanfar Hussain³**

¹*Department of Chemistry, NED University of Engineering. & Technology,
Karachi, 75270, Pakistan*

**Email: muhammadammar741@gmail.com*

Petrochemical water effluents possess significant amount of organic compounds. In the presented study, ozone has been employed as an oxidant to study the presence of organic compounds. For the purpose, petrochemical wastewater sample was collected from Pakistan refinery limited (PRL). COD and pH studies were conducted on collected wastewater by ozonation method. The samples after ozonation of 12 hours showed a significant COD reduction up to 80 %, whereas no change was observed in the pH of wastewater. Therefore, ozone treatment was observed to be an effective way for the COD control of petrochemical wastewater samples.

Key words: Petrochemical Wastewater, Ozonation, COD Ozonation, pH



Technical Session 07

Latest Research in Medicinal Chemistry



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IICC21-O-49	Internalization and Externalization Study of ^{99m}Tc-labeled Thymoquinone for Cancer Imaging Agent Using Rhabdomyosarcoma Cell Line Saima Tariq, Samina Roohi, <u>Syed Ali Raza Naqvi</u>
IICC21-O-50	Bacterial Biofilm Inhibition, Hemolytic and Structure-Activity Relationship of N-(2,3-Dihydro-1,4-Benzodioxin-6-yl)-4-Nitro-N-(Substituted-Benzyl)Benzenesulfonamides <u>Misbah Irshad</u>
IICC21-O-51	Mosquito Repellent and Larvicidal Activity of Lantana Camara Linn. <u>Anjum Ayub</u> , Sabira Begum, Rajput Muhammad Tariq
IICC21-O-52	Study of Antimicrobial Efficacy of Coal Extracted Humic Acid <u>Kiran Aftab</u> , Danial Khan, Ayesha
IICC21-O-53	Spectrophotometric Studies of Lawsonia L. Leaves Extract <u>Atya Hassan</u> , Adeel Shahid and Syed Haider Jafferery
IICC21-O-54	Furan Conjugated Tripeptide as Promising Anticancer Agent <u>Hunain Ali</u> , Almas Jabeen, Rukesh Maharjan, Muhammad Nadeem-ul-Haque, Husena Aamra, Salma Nazir, Serab Khan, Hamza Olleik, Marc Maresca, and Farzana Shaheen
IICC21-O-55	Ficus Carica Fruit for the Cure of Many Diseases: A Step Forward to Discover New Lead Compounds from Natural Plant Resources <u>Rabbia Irfan</u> , Somia Gul
IICC21-O-56	Investigation of Synergistic Effects of Commonly Used Antibiotics in Combination with Silver Nanoparticles Against Methicillin Resistant Staphylococcus Aureus <u>Zarlish Sultana</u>



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IICC21-O-49



Internalization and Externalization Study of ^{99m}Tc -Labeled Thymoquinone for Cancer Imaging Agent Using Rhabdomyosarcoma Cell Line

Saima Tariq¹, Samina Roohi¹, Syed Ali Raza Naqvi^{2*}

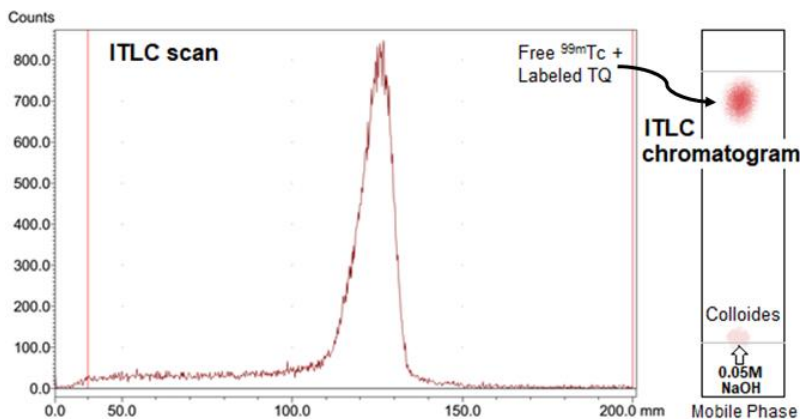
¹Isotope production division, Pakistan Institute of Nuclear Science and Technology, Nilore, Islamabad-Pakistan

²Department of Chemistry, Government College University, Faisalabad-38000, Pakistan

*E-mail: draliraza@gcuf.edu.pk

Thymoquinone (TQ) is a bioactive phytochemical isolated from *Nigella sativa*, has been investigated for biochemical and biological activities in both in-vitro and in-vivo models. It is best known for its anticancer activities. TQ accomplishes anticancer activities through targeting multiple cancer markers including PPAR- γ , PTEN, P53, P73, STAT3 and generation of ROS at cancer cell surface. The radiolabeling of thymoquinone with γ - and β -emitter radionuclide could be used as cancer diagnostic or therapeutic radiopharmaceutical, respectively. In this study we are reporting the radiolabeling of thymoquinone with ^{99m}Tc (a γ -emitter radionuclide), stability in saline and blood serum, internalization and externalization of ^{99m}Tc -TQ using rhabdomyosarcoma cancer cells line. The quality control study revealed more than 95% labeling yield and stable in blood serum up to 4 h. In-vitro internalization rate was recorded $27.08 \pm 0.95\%$ at 1 h post 120 min internalization period, which was slow comparatively slow or in agreement with the data reported in literature. The results of the study indicate that ^{99m}Tc -TQ could be investigated for further key pre-clinical parameters to enter Phase-I clinical trials.

Keywords: Thymoquinone, Phytochemical, Phabdomyosarcoma, Theranostic agent, Radiopharmaceuticals.



Highlights:

- Rhabdomyosarcoma is a skeletal muscles malignancy and it is common in most parts of the world
- Thymoquinone is recognized as an efficient natural product based chemotherapeutic agent for RMS.
- In this study the thymoquinone was labeled with ^{99m}Tc to study cell trafficking using RMS cell line to assess cancer imaging potential



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Bacterial Biofilm Inhibition, Hemolytic and Structure-Activity Relationship of N-(2,3-Dihydro-1,4-Benzodioxin-6-yl)-4-Nitro-N-(Substituted-Benzyl)Benzenesulfonamides

Misbah Irshad^{1*}

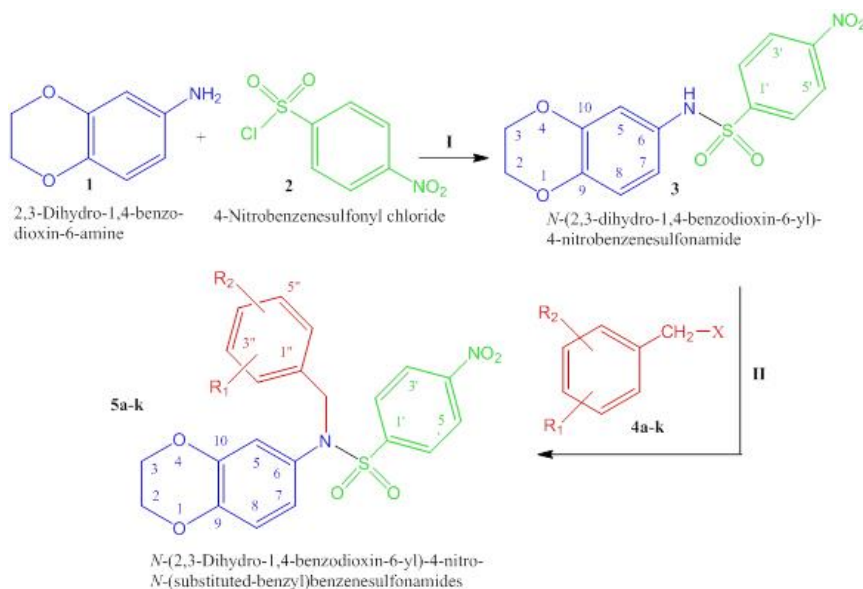
¹Department of Chemistry, Division of Science & Technology, University of Education, 54770-Lahore, Pakistan.

*E-mail: misbahirshad@ue.edu.pk

In the presented work the new antibacterial compounds 5a-k were fabricated that combine sulfonamide and benzodioxane fragments in their framework. All the molecules were synthesized in good yields and their structures were thoroughly corroborated by spectroscopic analysis. Some of the compounds displayed good antibacterial potential, particularly having monosubstituted benzyl ring which was imparted from benzyl halides 4a-k. Thus it was concluded from the structure-activity relationship that compound either bearing a small sized methyl group at *ortho*-position of benzylic moiety (5a) or the molecules having a halogen group at *ortho* or *meta*-position (5e, 5f, & 5j) generally behaved as suitable antibacterial agents against both strains. Thus these compounds 5a, 5e, 5f, and 5j exhibited suitable antibacterial potential against *Bacillus subtilis* and *Escherichia coli*, and also possessed mild cytotoxicity. On these bases, by modifying the structure in the given series the drug candidates could find their utility as suitable antibacterial agents.

Keywords: 1,4-Benzodioxine, 4-Nitrobenzenesulfonamide, Benzyl halides, Spectral analysis, Biofilm inhibition.

Graphical Abstract:



Highlights:

- (I) 10% Na₂CO₃/distilled water/stirring/4 hours.
- (II) DMF/LiH/Substituted-benzyl halides (4a-k)/stirring/RT/4-5 hours



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Mosquito Repellent and Larvicidal Activity of *Lantana camara* Linn

Anjum Ayub^{1*}, Sabira Begum², Rajput Muhammad Tariq³

¹Department of Chemistry, NED University of Engineering & Technology,
Karachi-75270, Pakistan

²H.E.J Research Institute of Chemistry, International Centre for Chemical and
Biological Sciences, University of Karachi, Karachi-75270, Pakistan

³Department of Zoology, University of Karachi, Karachi-75270, Pakistan
*E-mail: anjumayub@neduet.edu.pk

Lantana camara Linn. belongs to the family Verbenaceae commonly known as Lantana. It is native of tropical America, has been introduced in various countries. Different parts of the plant are used for the treatment of various human ailments such as eczema, bilious fever, swellings, ulcers, toothache, influenza, tumors, anemia, malaria and antiseptic for wound. Phytochemical studies undertaken by different groups of worker on different parts of the plant have resulted in the isolation of various flavonoids, steroids, and terpenoids. Mosquitoes transmit serious human diseases, causing millions of deaths every year. Use of insecticides to control vector mosquitoes has caused physiological resistance and adverse environmental effects. Several recent studies indicated that phytochemicals has a major role in mosquito control programme. In the light of these findings in the present investigations the methanolic extract, its fractions and pure compounds of *Lantana camara* were tested for mosquito repellent and larvicidal activities against dengue vector mosquito *Aedes aegypti*.

Keywords: *Lantana camara* Linn., Verbenaceae, Mosquito repellent, Larvicidal, *Aedes aegypti*



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Study of Antimicrobial Efficacy of Coal Extracted Humic Acid

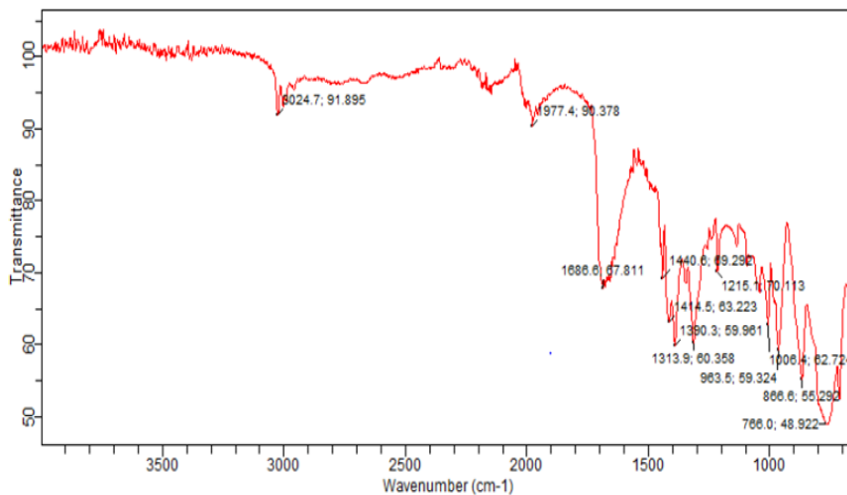
Kiran Aftab^{1*}, Danial Khan¹, Ayesha Riaz¹

¹Department of Chemistry, Government College University, Faisalabad

*E-mail: drkiranaftab@gcuf.edu.pk

To explore the non-fuel applications of high ash contented indigenous coal resources, the present study was carried out. The maximum observed yield of humic acid was 28.8% obtained by microwave assisted alkali (0.5 N KOH) extraction. Extracted humic acid showed E4/E6 value of 4.84 indicates high degree of condensation of aromatic humic components. The FTIR spectra of coal and coal extracted humic acids showed prominent absorption bands in the region of 3500-3700 cm⁻¹, 2850-3100 cm⁻¹, 1700-1995 cm⁻¹ and 1301-1451 cm⁻¹ shows the presence of various oxygen containing functional groups like carboxyl, phenolic, hydroxyl group and benzene derivatives also. To evaluate the bio efficacy of extracted samples of humic acid in-vitro antimicrobial activity was studied against different pathogens. Against *Staphylococcus aureus* and *Bacillus cereus* strains of bacteria the observed minimum inhibitory concentration values were $\leq 125 \mu\text{g mL}^{-1}$ and $\leq 250 \mu\text{g mL}^{-1}$ respectively. In contrast, bacterial strain of *E. coli* showed resistance against this because this bacterial strain is ubiquitous in environment. The minimum inhibitory concentration values of $\leq 125 \mu\text{g mL}^{-1}$ against *Aspergillus niger* and $187.5 \mu\text{g mL}^{-1}$ against *Fasarium avanceum* fungal strain also show efficient antifungal activity. Thus, low grade coal extracted humic acid might be developed as a new type of antimicrobial agent.

Keywords: Low grade coal, Antimicrobial activity, Humic acid, Disc diffusion method.



Highlights:

- For effective yield of humic substances the method development
- Extracted humic acid sample showed close resemblance with standard humic acid
- Extracted humic acid may be a potential candidate against pathogens



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Spectrophotometric Studies of *Lawsonia inermis* Leaves Extract

Atya Hassan^{1*}, Adeel Shahid², Syed Haider Jafferery¹

¹Department of Chemistry Federal Urdu University Arts Science & Technology
Gulshan Campus Karachi, Pakistan

²Department of Applied Chemistry, Government College University, Faisalabad

*Email: atiya.hassan@fuuast.edu.pk

This study is focused the phytochemical study of the extraction of *Lawsonia inermis* (Heena leaves) at room temperature $30 \pm 1^\circ\text{C}$. The extract hue of *Lawsonia inermis* was dark brown colour in aqueous medium and light orange in ethanol solvent at room temperature $30 \pm 1^\circ\text{C}$. The λ_{max} range of this dye was observed at 640 to 700nm. It contains Laswsone as active compound, it is responsible for the dye color. However, the effect of different percent solutions of extracted dye in the absorbance in both aqueous and non-aqueous medium were studied. The linear trend was obtained which reflects that the absorbance was gradually increased by increasing the different % solutions dyes. Decolourization phenomena was also reported in presence and absence of light in ethanolic solvent system. Linear behavior against the pH and conductance were obtained with different % solutions of dyes as well as at different time interval. All these investigation was done pH-metry, conductometry and spectrophotometry.

Keywords: Phytochemical, *Lawsonia inermis*, Absorbance, pH-metry, conductometry and Spectrophotometry.



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Furan Conjugated Tripeptide as Promising Anticancer Agent

Hunain Ali¹, Almas Jabeen², Rukesh Maharjan¹, Muhammad Nadeem-ul-Haque¹, Husena Aamra¹, Salma Nazir¹, Serab Khan¹, Hamza Olleik^{3,4}, Marc Maresca^{3*}, Farzana Shaheen^{1*}

¹H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan

²Dr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan

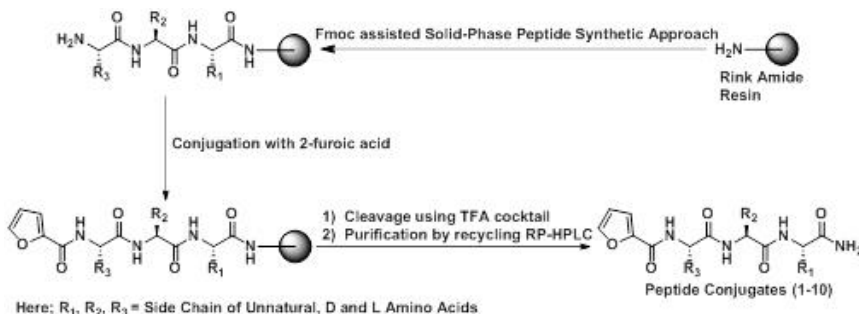
³Aix Marseille Univ., CNRS, Centrale Marseille, iSm2, 13397 Marseille, France

⁴Department of Biology, American University of Beirut, Lebanon

*E-mail: afnan.iccs@gmail.com, m.maresca@univ-amu.fr

Heterocyclic compounds are very important pharmacophores and unique scaffold in drug discovery. Peptides conjugated with heterocycles are important medicinal agents. Tripeptides conjugated with a furoyl moiety at C-terminal were reported to inhibit protease enzymes with greater selectivity and enhanced effectiveness and also possessed antineoplastic activity. Furan-capped tripeptides containing unusual residues such as 4-hydroxyphenylglycine were reported to exhibit protease inhibition activity against dengue virus (DENV) and West Nile virus (WNV). In the current study, a peptide library (furan conjugated peptides **1-10**) was synthesized using Fmoc-assisted solid-phase peptide methodology which leads to the identification of a potent furan conjugated peptide (**4**) as selective anticancer agent against HeLa cancer cell lines. This study revealed a good structure-activity relationship among various peptide conjugates. Peptide conjugate **4** in its branched form was found to be inactive. AFM and staining with rhodamine 123 and propidium iodide showed membranolytic effect of peptide conjugate **4** [1].

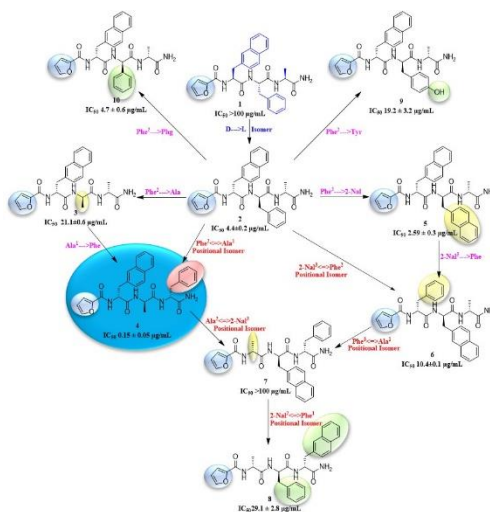
Keywords: Peptide conjugates, Heterocycles, Furan-based tripeptides, HeLa cancer cell lines, Structure-activity relationship.



References: Ali, H.; Jabeen, A.; Maharjan, R.; Nadeem-ul-Haque, M.; Aamra, H.; Nazir, S.; Khan, S.; Olleik, H.; Maresca, M.; Shaheen, F. Furan-Conjugated Tripeptides as Potent Antitumor Drugs. *Biomolecules* 2020, 10, 1684 (<https://doi.org/10.3390/biom10121684>).

Highlights:

- Peptide library (furan conjugated peptides **1-10**) was synthesized using Fmoc-assisted solid-phase peptide methodology.
- Structure-activity relationship among various peptide conjugates was developed.
- Furan conjugated peptide (**4**) was identified as selective anticancer agent against HeLa cancer cell lines.
- AFM and staining with rhodamine 123 and propidium iodide showed membranolytic effect of peptide conjugate **4**.





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IICC21-O-55



***Ficus carica* Fruit for the Cure of Many Diseases: A Step Forward to Discover New Lead Compounds from Natural Plant Resources**

Rabbia Irfan¹, Somia Gul^{1*}

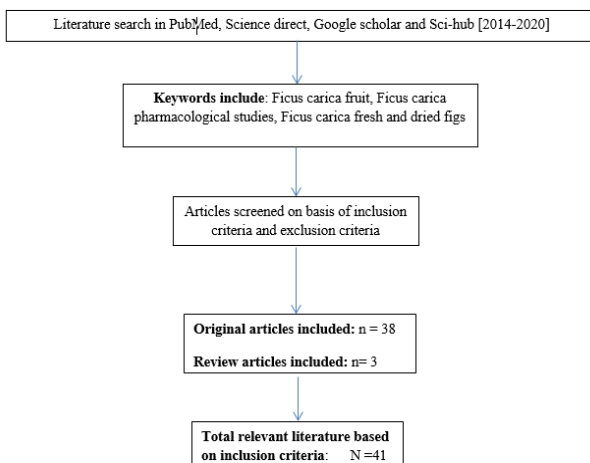
¹Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Jinnah University for Women, Karachi, 74600, Pakistan

*E-mail: drsomi1983@yahoo.com

Ficus carica Linn is one of the oldest traditional cultivate plant indigenous to Mid-East and West Asia region. Every part of *Ficus carica* plant has of great medicinal value as different parts contains different bioactive compounds which constitutes their medicinal therapeutic and health promoting activities. The aim of the current study was to gather the information of *Ficus carica* fruit (both fresh and dried ripened fruit) regarding its taxonomy, phytochemicals, nutritional contents, pharmacological activities and toxicology to check its potential for discovery of lead compounds of plant origin. The information regarding *Ficus carica* fruit searched in PubMed, Science direct, Google scholar and Sci-hub from the year 2014 to 2020. It is concluded that *Ficus carica* fruit is found as rich source of phytochemicals mainly anthocyanins and polyphenols. Anthocyanins (and its recently developed derivatives) are highly beneficial for human health as prevent cardiac diseases and cancer and in plants provide defense against environmental stress. While polyphenols by their anti-oxidant properties prevent number of other diseases. These discoveries provide new insight for pharmaceutical industries to manufactured drugs from natural origin, act as potent therapeutic agent, produce less side effects and provide great economical values to pharmaceutical industries as well as to country.

Keywords: *Ficus carica* fruit, Fig seeds, Phytochemical activities, Multi drug Resistance, Anthocyanins and polyphenols

Graphical abstract



Highlights:

- *Ficus carica* fruit is found as rich source of phytochemicals mainly anthocyanins and polyphenols.
- Discovered Anthocyanins are highly beneficial for human health as prevent cardiac diseases and cancer and polyphenols by their anti-oxidant properties prevent number of other diseases.
- These discoveries provide new insight for pharmaceutical industries to manufactured drugs from natural origin, act as potent therapeutic agent, produce less side effects and provide great economical values to pharmaceutical industries as well as to country.



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IICC21-O-56



Investigation of Synergistic Effects of Commonly Used Antibiotics in Combination with Silver Nanoparticles Against Methicillin Resistant *Staphylococcus aureus*

Zarlish Sultana^{1*}

¹Department of Microbiology Kohat University of Science & Technology, Khyber Pakhtunkhwa, Pakistan

*Email: gullish01@gmail.com

Silver nanoparticles are known for their antimicrobial properties are used extensively in various medical and general applications. In this study, the combination of silver nanoparticles and the conventional antibiotics e.g. ampicillin and ceftriaxone were tested against MRSA. The MIC and fractional inhibitory concentration index (FICI) were determined to confirm antibacterial susceptibility and synergistic effects. The results showed that silver nanoparticles possessed antibacterial effects and synergistic activities. The resistance to antibiotic against MRSA has become a serious problem. In our study different doses and different concentration of ampicillin and ceftriaxone were used in broth microdilution method and checkerboard assay. The results showed that these drugs consist of antibacterial activity and their doses were reduced. Silver nanoparticles with combination of these drugs in some ratios reduced the resistance which is the most emerging problem nowadays. Experiments were conducted and MIC of ampicillin alone was $187.5 \mu\text{g L}^{-1}$ and with combination of Nano particles $7.8125 \mu\text{g L}^{-1}$ FIC of drug and nano particles was .25 and .25 respectively Σ FIC was 0.5. Similarly MIC of ceftriaxone alone was $7.8125 \mu\text{g L}^{-1}$ and MIC of nanoparticle was $7.8125 \mu\text{g/l}$. FIC of ceftriaxone and nanoparticles was 0.5 and 1 and Σ FIC 1.5. When FIC value is greater than 0.5 then the combination shows synergistic effect. The development of resistance is almost an evitable consequence of clinical use of antimicrobial drugs. However it can be controlled by continued surveillance, infection control procedures and improved antibiotic usage. Strict control on the use of antibiotics and appropriate measures against over the counter availability and self-medication is recommended.

Keywords: Silver, MRSA, Ceftriaxone, Antibacterial.



Technical Session 08

Trends in Synthetic Chemistry



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IICC21-O-57	<p>Synthesis, Molecular Docking, Dynamic Simulations, Kinetic Mechanism, Cytotoxicity Evaluation of Heterocyclic Scaffolds as Promising Pharmacological Agents</p> <p><u>Syed Adnan Ali Shah</u>, Muhammad Taha, Muhammad Athar Abbasi, Aziz-ur-Rehman, Zainul Amiruddin Zakaria</p>
IICC21-O-58	<p>Synthesis and Characterization of Oximes Exhibiting Antibacterial Activity</p> <p><u>Hamid Ullah</u>, Abdul Haleem, Riffat Ullah, Anjum Ayub, Dildaraz Khan, Shafiullah Khan</p>
IICC21-O-59	<p>Greening the Blue: Biological Synthesis, Fabrication and Characterization of Polymer Based Antibacterial Nanocomposites Using Metabolic System of <i>Aspergillus Fumigatus</i></p> <p><u>Asma Ansari</u>, Sadaf Raza, Afsheen Aman</p>
IICC21-O-60	<p>Synthesis, Conformational, Cytotoxicity and Anti-Inflammatory Studies of the Orbitide [1-8-NaC]-Zanriorb A1 and Analogs</p> <p><u>Muhammad Nadeem-ul-Haque</u>, Anila Bashir, A. Ganesan, Almas Jabeen, M. Iqbal Choudhary, Farzana Shaheen</p>
IICC21-O-61	<p>Facile One Pot Synthesis of Short Chain Ethyl 6-Methyl-4-Phenyl-2-Thioxo-1,2,3,4-Tetrahydropyrim-Idine-5-Carboxylate Stabilized Silver Nanoparticles as Promising Nano-Hybrid with Potential Impact in Environmental and Biological Applications</p> <p>Rafia Usman Khan, Nuzhat Arshad, Jamshed Hashim, Razia Sultana, <u>Zain Ahmed Shah</u>, Waqas Zaidi, Haniya Sheikh, Samar Khan</p>
IICC21-O-62	<p>Solid-Phase Total Synthesis of Marine Natural Peptide Styliissamide G</p> <p><u>Farkhanda Mushtaq</u>, Farzana Shaheen</p>
IICC21-O-63	<p>A Facile Method to Access Humic Acid from Soil Under Alkaline Environment and its Application on Mustard (<i>Brassica compestris</i>) and Wheat (<i>Triticum indicum</i>) Seeds Germination</p> <p><u>Tajnees Pirzada</u>, Weenghar Ali Chandio, Mir Munsif Ali Talpur1, Abdul Majid</p>
IICC21-O-64	<p>Biosynthesis and Structural Characterization of an Exopolysaccharide Produced by <i>Zymomonas Mobilis</i></p> <p><u>Rabeeya Iftikhar</u>, Asma Ansari, Nadir Naveed Siddiqui, Fayaz Hussain, Afsheen Aman</p>



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Synthesis, Molecular Docking, Dynamic Simulations, Kinetic Mechanism, Cytotoxicity Evaluation of Heterocyclic Scaffolds as Promising Pharmacological Agents

Syed Adnan Ali Shah^{1,2*}, Muhammad Taha³, Muhammad Athar Abbasi⁴, Aziz-ur-Rehman⁴, Zainul Amiruddin Zakaria^{5,6}

¹*Faculty of Pharmacy, Universiti Teknologi MARA, Cawangan Selangor Kampus Puncak Alam, 42300 Bandar Puncak Alam, Selangor Darul Ehsan, Malaysia*

²*Atta-ur-Rahman Institute for Natural Product Discovery, Universiti Teknologi MARA, Cawangan Selangor Kampus Puncak Alam, 42300 Bandar Puncak Alam, Selangor D. E., Malaysia*

³*Department of Clinical Pharmacy, Imam Abdulrahman Bin Faisal University, Dammam, Saudi Arabia*

⁴*Department of Chemistry, Government College University, Lahore, Pakistan*

⁵*Department of Biomedical Science, Universiti Putra Malaysia, UPM Serdang, Selangor 43400, Malaysia*

⁶*Integrative Pharmacogenomics Institute (iPromise), Universiti Teknologi MARA Cawangan Selangor Kampus Puncak Alam, Bandar Puncak Alam, Selangor 42300, Malaysia*

**E-mail: syedadnan@uitm.edu.my*

Many heterocyclic compounds are distinguished as active products pharmaceutically and are gaining consistent attention in the development of new active multifunctional drugs candidates. Heterocyclic molecules have various clinical applications and play an active role as antitumor, antibacterial, anti-inflammatory, antiviral, and antifungal agents. Current study deals with the synthesis and biological screening of benzofuran-based-thiazolidinone analogues, diindolylmethane (DIM), thiophene-based derivatives of Benzimidazole-Based Analogs and 1,2,4-triazole scaffolds for their in-vitro anticancer, in vitro antioxidant evaluation, α -glucosidase, urease, tyrosinase inhibitory activities. All analogues exhibited excellent to good enzyme inhibitory potentials and also exhibited the potent anticancer activity against HCT116 cell lines. Structure-



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activity relationship (SAR) has been established on the basis of electronic effects and position of different substituents present on phenyl ring. In order to rationalize the binding interactions of most active analogues with the active site of enzyme, molecular docking study was conducted. Molecular docking evaluations envisaged their binding within the active region of enzyme with good docking energy values.

Keywords: Heterocyclic compounds, Benzofuran, Benzimidazole, Enzyme inhibitory activities, molecular docking study.



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IICC21-O-58



Synthesis and Characterization of Oximes Exhibiting Antibacterial Activity

**Hamid Ullah^{1*}, Abdul Haleem¹, Riffat Ullah², Anjum Ayub³,
Dilfaraz Khan², Shafiullah Khan²**

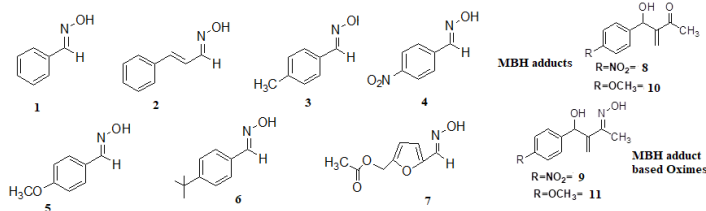
¹Department of Chemistry, Balochistan University of Information Technology,
Engineering and Management Sciences, Quetta 87300, Pakistan

²Institute of Chemical Sciences, Gomal University, D I Khan, KPK, Pakistan

³Department of Chemistry, NED University of Engineering and Technology,
Karachi, Pakistan

*E-mail: hamidullah9@gmail.com; hamid.ullah@buitms.edu.pk

Oximes and related compounds are organic substances bearing “C=N-OH” functionality. They are reported for their high structural diversities and strong biological activities. Chemically they can be transformed into almost all classes of organic compounds and inorganic complexes. The various chemical and biological significances justify oximes as attractive structures for scientists. In the present research a series of aldoximes were prepared by treatment of the different aldehydes with $\text{NH}_2\text{OH}\cdot\text{HCl}$ under stirring and at room temperature upto 60°C . To obtain MBH adduct based ketoximes, initially MBH adducts were prepared as precursors which were then subjected to oximation. All the products were concentrated on rotary evaporator and then purified chromatographically. As a result a series of structurally diverse aldoximes and MBH adduct keto oximes were obtained in good to the excellent yield (70-92%) are shown in figure. All the oximes were characterized through respective spectral analysis and performed antibacterial activity.

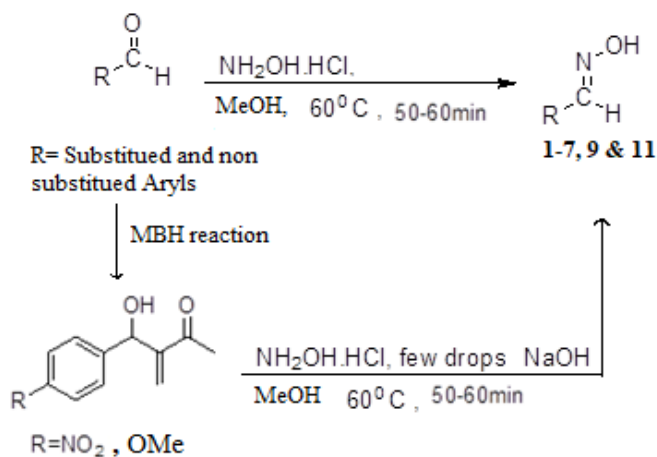


Keywords: Aldehydes, MBH reaction, MBH adducts, Oximation, Oximes .

Acknowledgement: ORIC BUITEMS for financial grant number # 01/Research Projects/ORIC/BUITEMS/2011/610.

References:

1. Ghazlojeh N. P., Setamdideh D. Orient. J. Chem., 31, 1823-1825 (2015).
2. Ullah H., Ferreira A.V., Bendassolli J. A., Rodrigo M. T., Formiga A., Coelho F., Synth. 47, 113-123(2013).



Highlights:

- Aldehydes were directly converted to oximes
- Aldehydes were used to prepare MBH adducts as precursors which were subsequently converted into respective oximes
- All the oximes were investigated for their antibacterial activity



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Greening the Blue: Biological Synthesis, Fabrication and Characterization of Polymer Based Antibacterial Nanocomposites Using Metabolic System of *Aspergillus fumigatus*

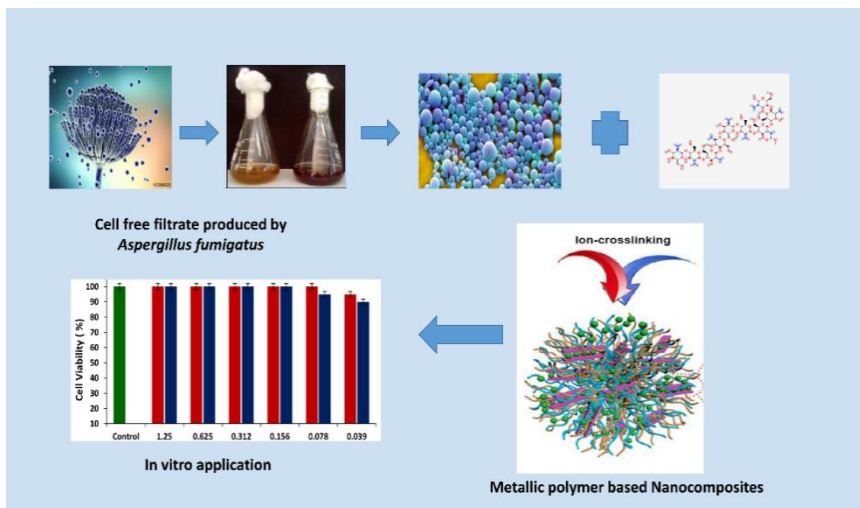
Asma Ansari^{1*}, Sadaf Raza¹, Afsheen Aman¹

¹Dr. Abdul Qadeer Khan Institute of Biotechnology and Genetic Engineering,
University of Karachi, Pakistan.

*E-mail: asansari@uok.edu.pk

Biosynthesis of nanomaterials have become a major interest in the field of nanotechnology. Nanoparticles have an emerging application in drug delivery system due to the target specificity and less reactive. Among a variety of nanoparticles, metallic nanoparticles especially silver nanoparticle and silver-based nanocomposites have dual advantage in targeted drug delivery and antimicrobial effect. Conventionally, nanoparticle synthesis requires chemical treatment to synthesize nanoparticles. Herein, the study focuses on the synthesis of silver nanoparticles using fungal metabolic system and the development of silver nanocomposites. The biosynthesized nanoparticles and the developed nanocomposites were characterized using advanced analytical techniques including UV-Vis spectroscopy, Scanning Electron Microscope, energy dispersive X-ray, dynamic light scattering, and Fourier transform infrared spectroscopic techniques. The biologically mediated silver nanoparticles are highly dispersed in nature with an average size and Zeta potential of 05 nm and -22.1 mV respectively. Both entities exhibited antimicrobial potential against pathogenic microbes. Fractional inhibitory concentration index of the developed silver-chitosan based nanocomposite confirmed its synergistic behavior against various bacterial species with no cytotoxic effect on mouse fibroblast cell lines. This fabricated nanocomposite system exhibited broad antibacterial spectrum that may help in future to design an alternative nanocarrier approach in order to control the emerging cases of MDROs.

Keywords: Chitosan, Silver, Nanoparticles, Nanocomposites, Non cytotoxic.



Highlights:

- Biosynthesis of Silver nanoparticles using *Aspergillus fumigatus*.
- Fabrication and characterization of polymer based nanocomposites.
- *In vitro* application of both nanoparticles and nanocomposites.



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Synthesis, Conformational, Cytotoxicity and Anti-Inflammatory Studies of the Orbitide [1-8-NaC]-Zanriorb A1 and Analogs

**Muhammad Nadeem-ul-Haque^{1*}, Anila Bashir¹, A. Ganesan³,
Almas Jabeen², M. Iqbal Choudhary^{1,2,4}, Farzana Shaheen¹**

¹H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan

²Dr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan

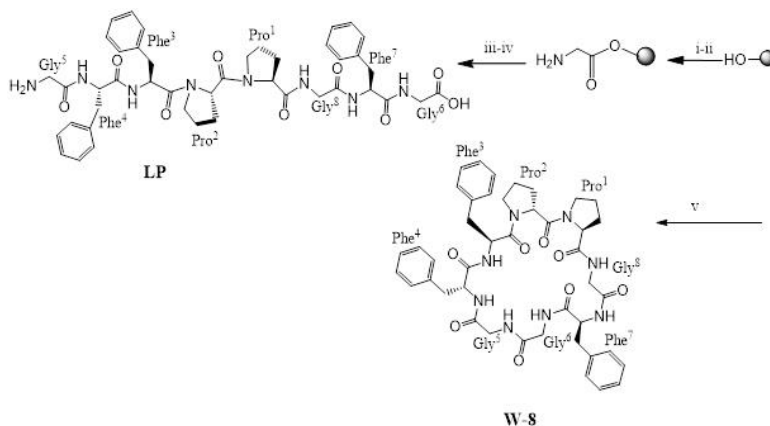
³School of Pharmacy, University of East Anglia, Norwich Research Park, Norwich NR4 7TJ, United Kingdom

⁴Department of Biochemistry, Faculty of Science, King Abdulaziz University, Jeddah-21412, Saudi Arabia

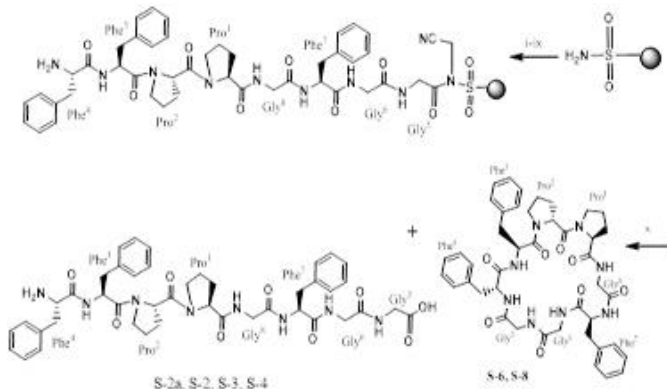
*Email: nadeem.and.chem@gmail.com

A new orbitide [1-8-NaC]-zanriorb A1 (1) was identified from a medicinal plant *Zanthoxylum riedelianum* as a potent apoptotic agent against Jurkat leukemia T-cells (IC₅₀ = 218.0 nM). Here we attempted the total syntheses of zanriorb A1 (1) on solid phase by two different routes and analogs of natural product (1). In the route A, the linear precursor (LP) of zanriorb A1 (1) was synthesized on solid phase, followed by solution-phase cyclization of LP which furnished the inseparable rotamers (W-8) of natural product (1). Second route B employed the complete synthesis of natural product (1) on solid phase via on-resin macrocyclization. The cyclic product S-6 obtained from route B was also found to be inseparable mixture of rotamers of natural product (1). A minor conformer S-8 was also obtained with some differences in chemical shifts from natural product (1). Interestingly, the second route also afforded unexpected linear precursor S-2a of natural product (1). To further confirm the linear sequence of S-2a, it was re-synthesized on Wang resin which afforded three peptide conformers 1a, 1b, and 1a-4 having same molecular ion peak as that of S-2a. Among these conformers, 1a was found to have same retention time as S-2a with both proline residues in *trans* configuration as in S-2a. All cyclic conformers

as well as the linear precursors of natural product (1) and cyclic analogs were found to be inactive against Jurkat leukemia T-cells, MCF-7 breast cancer and 3T3 murine fibroblast cell lines. Linear precursor S-2a of natural product (1), cyclic analog CP-2, and CP-4 potently inhibited nitric oxide (NO.) at ($IC_{50} = 88.1 \pm 2.2 \mu M$), ($IC_{50} = 65.0 \pm 3.5 \mu M$), and ($IC_{50} = 22.2 \pm 0.2 \mu M$) produced from LPS activated J774.2 macrophages as compared to nitric oxide standard inhibitor (L-NMMA, $IC_{50} = 97.5 \pm 3.2 \mu M$), while all other products were found inactive.

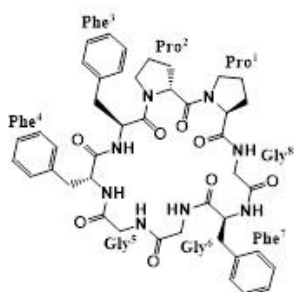


(SCHEME-1)



(SCHEME 2)

Keywords: Orbitides, Zanriorb A1, Solid-phase peptide synthesis, Proline rotamers, Apoptotic agent, Nitric oxide inhibition.



Natural Product Zanriorb A1

Active against Jurkat leukemia T-cells ($IC_{50} = 218.0 \text{ nM}$)

Synthetic route A

via solution-phase cyclization

W-8

Inactive conformational mixture of
zanriorb A1

Synthetic route B

via on-resin cyclization

(S-6 and S-8)

Inactive conformational mixture of zanriorb A1

+
Linear precursor (S-2a) of zanriorb A1 as potent
nitric oxide inhibitor

Highlights:

- Total synthesis of [1-8-N α C]-zanriorb 1A and Synthesis of analogs.
- Conformational and structural studies of synthetic conformers of natural product (1) from two routes by NMR-spectroscopy and MS/MS techniques.
- Biological studies of synthetic conformers of natural product (1) and analogs against anticancer cellines.



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Facile One Pot Synthesis of Short Chain Ethyl 6-Methyl-4-Phenyl-2-Thioxo-1,2,3,4-Tetrahydropyrim-Idine-5-Carboxylate Stabilized Silver Nanoparticles as Promising Nano-Hybrid with Potential Impact in Environmental and Biological Applications

Rafia Usman Khan^{1*}, Nuzhat Arshad¹, Jamshed Hashim²,
Razia Sultana³, Zain Ahmed Shah¹, Waqas Zaidi¹,
Haniya Sheikh¹, Samar Khan¹

¹ NED University of Engineering & Technology, Karachi, Pakistan

² HEJ Research Institute of Chemistry, ICCBS, University of Karachi, Pakistan

³ Applied Chemistry Research Center PCSIR Laboratories, Pakistan

*Email: rkhan@neduet.edu.pk

Short chain heterocycle thiol Ethyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrim-idine-5-carboxylate (DHPMs), stabilized silver nanoparticles (AgNps) were synthesized. (DHPMs) possess a single thiol group at the focal point which strongly stabilize the nascent AgNps. The size and distribution of the AgNps produced can also be correlated with the rate of Ag reduction. The short alkyl chain of (DHPMs) effectively controlled the growth kinetics and surface morphology of AgNps. The optical properties of the prepared AgNps were analyzed using Ultraviolet-visible spectroscopy, Fourier-transform infrared spectroscopy, Atomic Force Microscopy (AFM) were vividly demonstrated the specific size morphology of AgNps-DHPMs with an average size of 10± 1 nm. The AgNps- DHPMs demonstrated phenomenal catalytic activity and within one second it reduces 4-nitrophenol to 4-aminophenol in the presence of NaBH₄ under ambient temperature and pressure conditions, which followed the pseudo-first-order rate kinetics. Silver nanoparticles (AgNps) are well known to have antimicrobial ability, but very little is known about the effect of AgNps for enzyme inhibition activities. Our prepared AgNps-DHPMs were examined for urease inhibition activity. AgNps-DHPMs were found to be significantly active with IC₅₀ values between 40.3± 0.28 %. Our experiments will provide guidelines for designing efficient catalysts and stabilizing agents in the future.
Keywords: Silver nanoparticles, Ethyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrim-idine-5-carboxylate stabilizer, 4-nitrophenol



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Solid-Phase Total Synthesis of Marine Natural Peptide Stylissamide

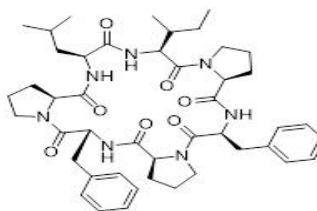
Farkhanda Mushtaq¹, Farzana Shaheen^{1*}

¹H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan

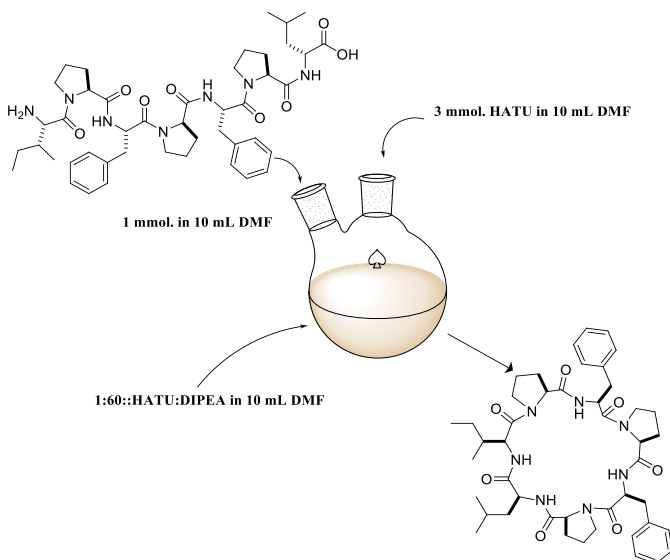
*E-mail: afnan.iccs@gmail.com

Cyclic peptides are structurally diverse classes of natural products. They are usually more conformationally rigid as compare to linear peptides, hence they are more potent in terms of selectivity and potency which makes them more preferable drug candidate. Cyclic peptides containing one or more proline residues provide more rigidity to the cyclic structure, enhancing their biological potential. Multiple proline rich cyclic peptides were reported to be isolated from various marine organisms. Stylissamide G, a new natural cycloheptapeptide was isolated and identified from the bahamian sponge *Stylissa caribica*. It is one of the proline rich cyclic peptide and was reported to show anthelmintic activities. Usually, such biologically important peptides are required to obtain in larger amount but the main disadvantage of isolation of such peptides resulted in lower yields. But synthesis of such proline containing peptides is also little bit complicated as there are multiple possibilities of conformational restriction and isomers due to proline ring. Thus, the present study is focussed on the total synthesis of this cyclic peptide and identification of its main conformational isomer responsible for its biological potential. Solid-phase peptide synthesis was used to synthesize linear precursor followed by solution phase cyclization. Its structure was confirmed by HRESIMS and NMR spectroscopic data.

Keywords: Marine cyclic peptides, Stylisamide G, Proline rich peptides, *Stylissa caribica*, Total synthesis.



Stylissamide G



Highlights:

- Stylyssamide G was synthesized by using a combination of solid and solution-phase Fmoc-assisted peptide methodology.
- The crude cyclic product was purified by RP-HPLC and confirmed by HRESIMS spectroscopy and NMR studies.



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A Facile Method to Access Humic Acid from Soil Under Alkaline Environment and its Application on Mustard (*Brassica campestris*) and Wheat (*Triticum indicum*) Seeds Germination

Tajnees Pirzada^{1*}, Weenghar Ali Chandio¹, Mir Munsif Ali Talpur¹, Abdul Majid²

¹*Institute of Chemistry, Shah Abdul Latif University, Khairpur, Sindh, Pakistan.*

²*Department of Biochemistry, Shah Abdul Latif University, Khairpur, Pakistan*

**Email: tajnees@yahoo.com*

The soil humic acid investigated in this study was conventionally isolated from agriculture lands of Khairpur Sindh by IHSS method and spectral features obtained by using various techniques such as X-ray diffraction, Fourier transform infrared (FTIR), UV-Vis spectroscopy and scanning electron microscopy (SEM). The results show that the isolated HA is rich in carboxylic and phenolic groups which contribute most to surface charge and reactivity of humic substances. Finally, HA effects were investigated on the seed germination profile including root and shoot length, mortality and fresh and dry weight of Mustard (*Brassica campestris*) and wheat (*Triticum indicum*) by applying different concentrations of HA (0, 5, 10, 15, and 20ppm) to the seeds of both plants. It was observed that application of HA at all levels improved the seed germination process but at 5ppm concentration significant increase in fresh and dry weight, shoot and root length appeared. Hence the application of lower concentration of HA could be more beneficial for the enhancement of germination process of Mustard and wheat plants. Spectroscopic analysis data obtained depicts the nature of isolated HA and its positive effects on the plants growth were confirmed. Now further research may be conducted for more insight information about mechanism and effects of HA on other plants.

Keywords: Humic acid, spectroscopic techniques, agriculture soil and germination.



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Biosynthesis and Structural Characterization of an Exopolysaccharide Produced by *Zymomonas mobilis*

**Rabeeya Iftikhar¹, Asma Ansari¹, Nadir Naveed Siddiqui¹,
Fayaz Hussain², Afsheen Aman^{1*}**

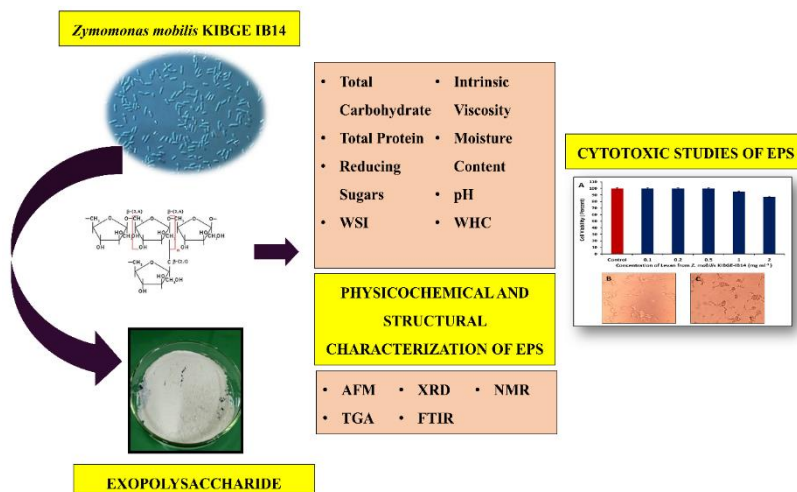
¹The Karachi Institute of Biotechnology & Genetic Engineering (KIBGE),
University of Karachi, Karachi-75270, Pakistan.

²Department of Materials Engineering, NED University of Engineering and
Technology, Karachi-75270, Pakistan.

*E-mail: afaman@uok.edu.pk

Exopolysaccharides (EPS) are produced by a range of bacterial, algal and fungal species. Amongst them, EPS of bacterial origin have exhibited more bioactive functionalities. Current study deals with the exploration of bacterial species that can produce EPS. Indigenously produced EPS was identified and characterized using different physicochemical and analytical techniques. Maximum yield of exopolysaccharide (44.7 gL⁻¹) was attained after 72 hours of incubation at 30°C under shaking conditions (180 rpm) when the culture medium was supplemented with 150.0 gL⁻¹ of sucrose. This exopolysaccharide displayed high water solubility (96.0 %) with low water holding capacity (17.0 %) and an intrinsic viscosity of about 0.447 dL g⁻¹. It exhibited a characteristic linear homopolysaccharide structure of levan when characterized using Atomic Force Microscopy (AFM), Thermogravimetric analysis (TGA) and X-Ray Diffraction (XRD), Fourier Transform Infrared (FTIR) and Nuclear Magnetic Resonance (NMR) spectroscopy. Cytotoxicity of different concentrations of levan was investigated against murine fibroblast cell lines and it was noticed that a higher concentration of levan (2.0 mg mL⁻¹) permitted the normal cell growth of NIH/3T3 cell lines. This non-cytotoxic and biocompatible nature suggests that this levan has the capability to be utilized in food, medical and other commercial industries.

Keywords: Exopolysaccharide, Levan, *Zymomonas mobilis*, Cytotoxic Analysis.



Highlights:

- The microbial source was used to produce an exopolysaccharide.
- This exopolysaccharide was characterized using advanced analytical techniques.
- This exopolysaccharide has potential to use in food industry.



Technical Session 09

Chemistry for Industrial Sustainability-III



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IICC21-O-65	Poly (Propylene Glycol) Bis(2-Aminopropyl) Ether (POPDA) Hardener Based Smart Glass Technology Use to Virus Covid-19 Challenges <u>Mujtaba Ellahi</u> , Muhammad. Furqan Ali, Adnan Murad Bhayo, Kashif Hussain Mangi
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IICC21-O-67	Synthesis of Eco-Friendly Polyethylene Terephthalate (PET) <u>Suraiya Jabeen</u> , Kehkashan Khan, Shagufta Ishteaque
IICC21-O-68	Use of Hydroxypropylated Barley Starch as Partial Casein Replacer in Preparation of Imitation Mozzarella Cheese <u>Tooba Mehfooz</u> , Tahira Mohsin Ali, Abid Hasnain
IICC21-O-69	Optimization and Genetic Characterization of Selected Bacteria for Biosurfactant Production Isolated from Oil-Contaminated Sites of Karachi <u>Faiza Anwar Ansari</u> , Erum Shoeb
IICC21-O-70	Production and Optimization of Self-Healing Concrete by Using Indigenous Bacteria <u>Muhammad Umar Bin Aamir</u> , Kashif Ahmed, Muhammad Aslam Bhutto
IICC21-O-71	Natural Dyeing of Cotton & Wool Fiber Using Bio-Mordant for Sustainable Development Sajid Ali, Aresha Ali Khan, Muhammad Kashif Pervez, Farman Ahmed, Muhammad Ali Versiani, <u>Rajkumar Dewani</u> , Kehkashan Khan



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IICC21-O-73	Synthesis of Nanosensors and Evaluation of Their Applications in Aqueous and Blood Samples. <u>Farhat Ikram</u> , Amtul Qayoom
IICC21-O-74	High Performance Liquid Chromatographic Method for Simultaneous Determination of Alprazolam with Antihistamines in Bulk Drug, Pharmaceutical Formulation and Human Serum <u>Shumaila Akram</u> , Saeeda Nadir Ali, Amtul Qayoom, Sajid Iqbal, Nida Naz, Inayatullah Memon
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IICC21-O-76	Self-organized Surfactant Assemblies as Nanostructured Dye Carriers: A Mixed Micellar Approach for Enhanced Dye Solubilization as an Application to Remove Dyes from Industrial Effluent by Micellar Enhanced Ultrafiltration <u>Muhammad Usman</u> , Amnah Yusaf
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IICC21-O-65



Poly (Propylene glycol) Bis(2-Aminopropyl) Ether (POPDA) Hardener Based Smart Glass Technology Use to Virus COVID-19 Challenges

**Mujtaba Ellahi^{1*}, Muhammad Furqan Ali², Adnan Murad
Bhayo³, Kashif Hussain Mangi⁴**

¹Advanced Polymer Science Laboratory, Department of Chemistry, Balochistan
University of Information Technology, Engineering and Management Sciences,
Quetta, Pakistan

²Department of Chemical Engineering, University of Karachi, Pakistan

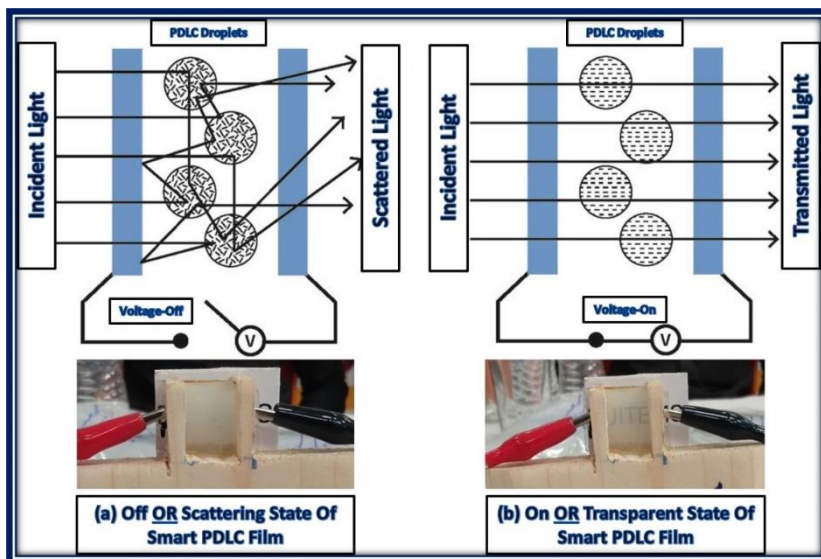
³Department of Chemistry and Chemical Biology, McMaster University,
Hamilton, Ontario L8S 4M1, Canada

⁴Michel Ange, Saint Nazaire, and University of Nantes, France

*E-mail: Mujtaba.ellahi@buitms.edu.pk

The current study designed to fabricate smart glass thin polymer dispersed liquid crystal (PDLC) films using with epoxy resin monomers/hardener/Nematic Liquid Crystal (NLCs) system. Refining strategies used for improving the stability and properties of smart PDLC films directly impact optical and electro-optical display panel performance. In this study, we have been arranged polymerization induced phase separation (PIPS) heat curing method to use the poly (propylene glycol) bis(2-aminopropyl) ether (POPDA) heat curing agent (Jeffamine D-230) hardener, Di-functional Ethylene glycol diglycidyl ether (EGDE) and tri-functional Trimethylolpropane triglycidyl ether (TMPTGE) epoxy resin of thin smart films by curing time 7 hour and at 90°C. The prepared smart glass panel films were characterized using liquid crystal device (LCD) parameters tester and scanning electron microscopy (SEM). The liquid crystal device technique and SEM confirm the interaction of TMPTGE monomer and POPDA hardener. The results of investigations of epoxy resins cured with POPDA depending on the feed ratio of epoxy monomers, the content of the curing agent, active diluents, and curing temperature. This smart glass technology will help to make a distance between the affected patients of COVID-19 and doctor as well as health care centres buildings, effected patient isolation rooms, hospitals, smart helmet, and smart mitigate social distances.

Keywords: Hardener, Epoxy resin, Liquid Crystal, Smart Glass, PDLC Films.



Highlights:

- To introduce the TMPTGE/EGDE/POPDA/NLCs thin films system in smart films glass technology
- POPDA depending on the feed ratio of epoxy monomers, the content of the curing agent
- Smart Glass Technology: An Innovative Way to Curb the Spread of COVID-19 challenges



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Development of Sun Protection Finish for Cotton Fabric Using Extracts of *Chenopodium album*

Faiza Nazir^{1*}, Ahsan Nazir^{2*}, Sharjeel Abid^{3*}

¹Department of Chemistry, Government College Women University Faisalabad

²National Textile University and National Textile Research Centre, Faisalabad

³Department of Textile Processing, National Textile University Faisalabad

*E-mail: faizanazir@gcwuf.edu.pk, ahsan.nazirr@gmail.com,
m.sharjeel.abid@gmail.com

The research work was aimed to investigate the ultraviolet protection factor (UPF) of *Chenopodium album*. Three different extracts of this plant were prepared in distilled water, methanol and n-hexane. In vitro spectrometric assay was employed to determine the sun protection factor (SPF) and ultraviolet protection factor. The antioxidant activity of extracts was determined by the radical scavenging ability by the usage of the stable radical DPPH. Total phenolic contents were determined by Folin Ciocalteu reagent using gallic acid as standard. Total flavonoids were determined by AlCl₃ method. Plant extracts were analysed by High performance liquid chromatography. Methanol extract of *Chenopodium album* showed the best results with highest yield as compared to aqueous and n-hexane extracts. While the UPF and SPF factors of methanol extract was also found to be maximum with highest antioxidant activity. The HPLC analysis of the plant extracts was performed which showed the methanol extract with higher contents of phenolic compounds that are also responsible for its maximum antioxidant activity.

Keywords: Sun protection factor, Medicinal plants, HPLC.



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Synthesis of Eco-Friendly Polyethylene Terephthalate (PET)

Suraiya Jabeen^{1*}, Kehkashan Khan², Shagufta Ishteaque³

¹*Institute of Environmental Studies, University of Karachi, Pakistan*

²*Department of Chemistry, Federal Urdu University, Karachi, Pakistan*

³*Department of Chemical Engineering, University of Karachi, Pakistan*

**E-mail: sujabeen@uok.edu.pk*

This study focuses to address global environmental pollution problem due to non-degradable plastic films. Though several countries have developed their own formulations from easily available cost effective raw materials but Pakistani researchers are still working for a commercialized product in collaboration of an industry. An extensively used natural polymer is starch because it is most plentiful available and low-cost too. Current methodology describes the development of improved formulation for the synthesis of cost effective and eco-friendly polyethylene terephthalate (PET). The prepared film will be analyzed for its tensile strength using Universal Testing Machine, thermal analysis, water absorption and biodegradability. The film preparation methods employed are polymer melting followed by extrusion blending and blow molding. Another alternative approach utilizing PET is to react polyethylene terephthalate-polyethylene glycol copolymer with starch in the presence of a coupling agent, viz. hexamethylenediisocyanate. The cost effective raw material would be blended with already available or even recycled PET films with naturally occurring degradable polymers to enhance their biodegradability, the developed product will impart a positive impact on economy too and there will be no more need of importing degradable packaging material. This will help in reducing the plastic pollution not only in Pakistan but globally too.

Keywords: Global environmental pollution, Improved formulations, Biodegradability, Polyethylene terephthalate



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Graphical Abstract:



Highlights:

- Plastic pollutions ubiquitous- Great Pacific Garbage Patch
- Solution-Biodegradable plastic
- Environmental Friendly Technique



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Use of Hydroxypropylated Barley Starch as Partial Casein Replacer in Preparation of Imitation Mozzarella Cheese

Tooba Mehfooz^{1*}, Tahira Mohsin Ali¹, Abid Hasnain¹

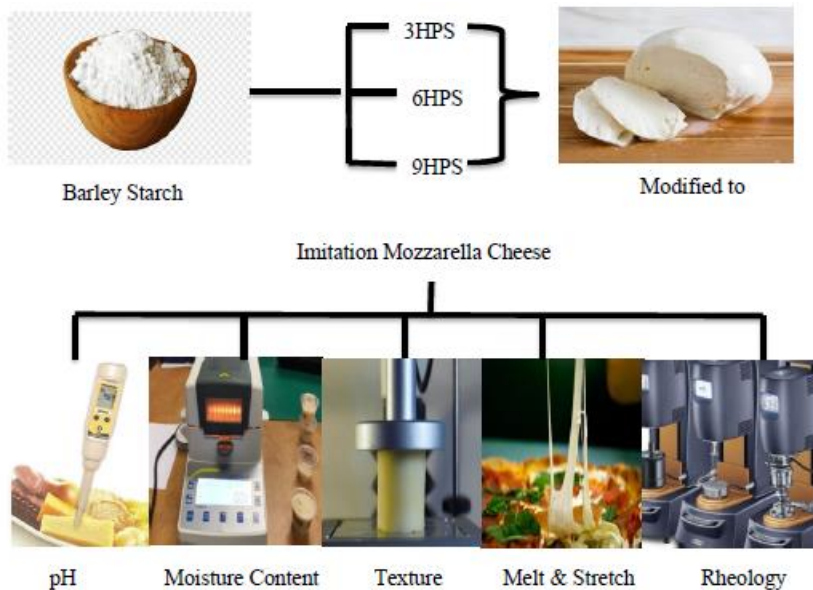
¹*Department of Food Science and Technology, University of Karachi, 75270, Karachi, Pakistan.*

**E-mail: toobamehfooz@gmail.com*

Mozzarella cheese imitates were prepared using native and hydroxypropylated barley starches. The extent of modification was 3%, 6% and 9%. Native barley starch cheese was denoted as NB and hydroxypropylated barely cheese were marked as 3HPS, 6HPS and 9HPS, respectively. In all the imitation cheese rennet casein was replaced with the aforementioned barley starches at a level of 15%. Improved melting characteristics were observed in case of native i.e. NB, 3HPS and 6HPS mozzarella cheese samples. Better stretch ability was observed in case of cheese prepared from hydroxypropylated barley starch than native and control. 9HPS cheese showed the most variation in rheological behaviour with no cross over temperature and least melt index as compared to other cheese samples.

Keywords: Mozzarella imitation cheese, Barley starch, Hydroxypropylated barley starch, Improved melt index.

Graphical Abstract:





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Optimization and Genetic Characterization of Selected Bacteria for Biosurfactant Production Isolated from Oil-Contaminated Sites of Karachi

Faiza Anwar Ansari^{1*}, Erum Shueb^{2*}

¹*Department of Genetics, University of Karachi, Pakistan.*

²*Department of Genetics, University of Karachi, Pakistan.*

**Email: faiza.ansari22@gmail.com, erumsh@uok.edu.pk*

Biosurfactants are amphiphilic compounds produced by living organisms, mostly on microbial cell surfaces or excreted extracellularly. Microorganisms that produce biosurfactant are isolated from sites that contaminated by petroleum hydrocarbons. The most important advantage of biosurfactants when compared to synthetic surfactants is their ecological acceptance. The present study is an attempt to optimize production of biosurfactant and protease simultaneously from bacterial isolates. Bacterially produced biosurfactant and proteases well known for many applications in various industries and due to their environmentally friendly nature. Isolates selected for biosurfactant production through oil spreading, hemolytic activity, CTAB agar plate, drop collapse test, BATH assay, and emulsification activity (E24). This study accomplishes that these isolates have the ability to produce commercially important biosurfactant and proteases respectively. It also suggested that apple pomace is a cost-effective substrate for the production of important biomolecules, these isolates have potential for future environmental friendly applications and suggest cost effective solution.

Key words: Biosurfactant, Cheap-carbon source, Arabian sea, Karachi coast



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ICC21-O-70



Production and Optimization of Self-Healing Concrete by Using Indigenous Bacteria

**Muhammad Umar Bin Aamir¹, Kashif Ahmed^{1*},
Muhammad Aslam Bhutto²**

¹*Department of Chemistry, Faculty of Industrial Chemistry, N.E.D. University of Engineering & Technology, Karachi, 75270, Pakistan.*

²*Department of Civil Engineering, Faculty of Civil and Infrastructure Engineering, N.E.D. University of Engineering & Technology, Karachi, 75270, Pakistan.*

**Email: Kashif25473@yahoo.com*

The current study aims to investigate the stability parameters with more emphasis on compressive strength, flexural strength, pullout strength for optimization and comparison of self healing concrete with conventional concrete. In this study bacterial species namely bacillus clausii, bacillus coagulans and lactobacillus reuteri were used as well as preparation of bacterial growth medium was also conducted. Thus results estimated shows higher compressive strength in case of bacillus coagulans based bacterial concrete specimens tested at 7 and 28 days of curing that is 31.85 % and 37.08% along with higher flexural strength for bacillus coagulans and bacillus clausii containing 22.6% and 23% increment respectively at 7 and 28 days of curing with higher pullout strength for lactobacillus reuteri containing 51.26 % and 38.25 % respectively. Moreover it can be concluded that the use of bacterial based concrete specimens will be advantageous to make it a life enriching and elegant construction material.

Keywords:

Self-Healing Concrete,
Microorganisms,
Optimization, Slant,
Curing





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Natural Dyeing of Cotton & Wool Fiber Using Bio-Mordant for Sustainable Development

Aresha Ali Khan¹, Sajid Ali¹, Muhammad Kashif Pervez^{2*},
Farman Ahmed^{3*}, Muhammad Ali Versiani¹,
Rajkumar Dewani², Kehkashan Khan^{1*}

¹Department of Chemistry, Federal Urdu University of Arts Science & Technology, Karachi, Pakistan

²Pakistan Council of Scientific and Industrial Research, Leather Research Centre, Karachi, Pakistan

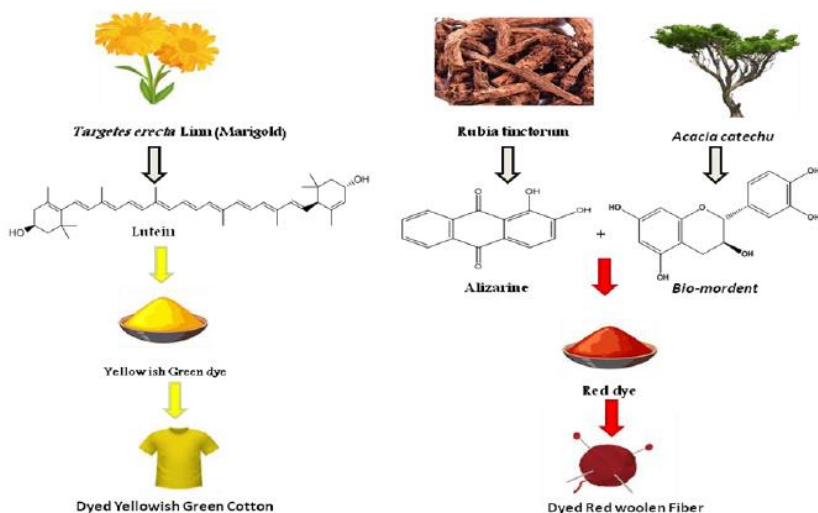
³Pakistan Council of Scientific and Industrial Research, Karachi Labs Complex, Karachi, Pakistan

*E-mail: sajidmeer136@gmail.com, rajdewaan@gmail.com

The synthetic dyes have been imported from other countries to Pakistan since long. This is not only a burden on our economy but there is a great concern of associated toxic effects too. Also, Metallic salts are used for complexation of dyes as well as mordant process. Most of the metallic salts create toxicity in the environment, human and in animal. The proposed investigation will be helpful to develop cost-effective and marketable dyes application utilizing indigenous natural resources with less or no toxic effects. Natural product-based dyes are a better replacement of synthetic dyes. In this study, some natural dyes are identified which can be used as an alternative of synthetic dyes. For instance, *Rubia cordifolia* (Madder root) upon treatment with *Acacia catechu* (a bio-mordant source) furnishes red hue. Wool fiber dyeing is also carried out using different mordanting methods to impart red tone into it. Similarly, lutein from *Tagetes erecta* Linn. (Marigold flower) impart greenish yellow shade to cotton. Bio-mordant with natural dyes can impart nearly same effect to wool & cotton fiber as metallic mordant link with synthetic dyes. These domestic natural dyes from Madder and Marigold will be cost-effective and eco-friendly with good dye stability.

Keywords: Natural dyes, Marigold, Madder, Bio-Mordant.

Graphical Abstract:



Highlights:

- Development of Cost-effective and Non-Toxic Dyeing
- Natural Product-based Dyes e.g. Marigold (*Rubia cordifolia*) and Madder (*Tagetes erecta* Linn)
- Bio-Mordant (*Acacia catechu*)



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An Efficient Process to Transform Phosphogypsum into Calcium Fluoride and Sulfate Ammonium

Yassine Ennaciri^{1*}, Mohammed Bettach¹

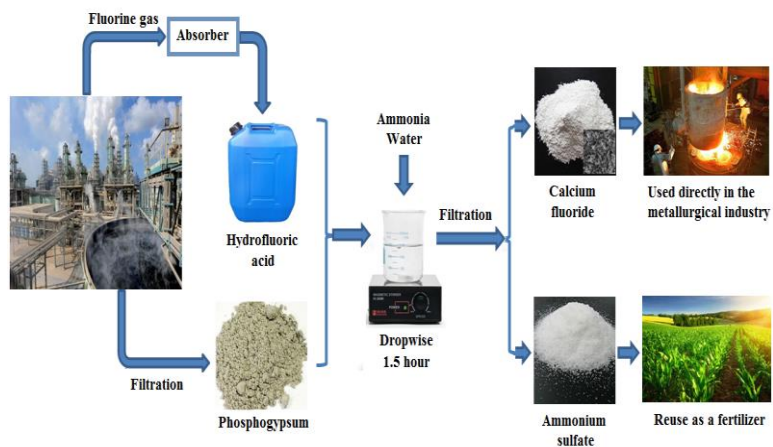
¹Department of Chemistry, Chouaib Doukkali University, El Jadida, Morocco.

*E-mail: yassinemaster@gmail.com

The wet process the phosphoric acid production from the digestion of phosphate rock by sulfuric acid gives rise to a by-product called phosphogypsum (PG), beside the emission of high fluorine into the atmosphere. Generally, a large quantity of this by-product is stockpiled or rejected without any pretreatment into environment. This management of PG may be caused several environmental problems in the long term. In this work, we proposed an efficient process permits to transform PG by the recycled hydrofluoric acid (HF) and ammonia (NH₃) into calcium fluoride (CaF₂) and ammonium sulfate ((NH₄)₂SO₄). Also, several technics (XRD, MEB, EDX, ICP) were applied to prove the quality of these obtained products. According to the obtained results, the produced CaF₂ and (NH₄)₂SO₄ can be used directly in the metallurgical industry and the agriculture respectively. In addition, this proposed process could be minimizing the PG rejection and the fluorine gas emission, and contributed to conserve the natural reserves of fluorite.

Keywords: Phosphogypsum, Calcium fluoride, Ammonium sulfate, Hydrofluoric acid, Ammonia.

Graphical Abstract:



Highlights:

- Efficient solution to the problems related to the phosphogypsum rejection
- The produced CaF_2 can be used directly in the metallurgical industry
- The obtained salt $(\text{NH}_4)_2\text{SO}_4$ is non-toxic and can be reused in agriculture



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Synthesis of Nanosensors and Evaluation of Their Applications in Aqueous and Blood Samples.

Farhat Ikram^{1*}, Amtul Qayoom¹

¹*Department of Chemistry, N.E.D. University of Engineering and Technology, Karachi, Pakistan.*

**E-mail: farhat@neduet.edu.pk*

Silver nanoparticles of flavonoid were synthesized and conjugation of silver was confirmed by FT-IR, UV-visible spectroscopy, MALDI-TOF and atomic force microscopy (AFM). To examine their potential and chemical sensing properties, different drugs and metal salt solutions were screened. In addition, sensing behavior when observed in the presence of commonly available metal ions and drugs then it was noticed that synthesized silver nanosensor has the property of sensing antibiotic and heavy metal ion simultaneously, while other interfering substances did not produce any change in the absorption intensity of nanoparticles. The synthesized nanoparticles were found to be drug selective, as no interference was observed upon addition of other drugs or metal ions. The sensing ability of synthesized nanoparticles towards one particular drug and heavy metal were checked in biological samples (plasma, serum) and environmental samples (tap water).

Keywords: Nanosensor; Sensing; Silver nanoparticles.



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High Performance Liquid Chromatographic Method for Simultaneous Determination of Alprazolam with Antihistamines in Bulk Drug, Pharmaceutical Formulation and Human Serum

Shumaila Akram^{1*}, Saeeda Nadir Ali², Amtul Qayoom², Sajid Iqbal³, Nida Naz⁴, Inayatullah Memon⁵

¹Department of Chemistry, University of Karachi, Pakistan

²Department of Chemistry, NED University of Engineering. & Technology

³Department of Chemistry, Jinnah Govt. College Nazimabad, Karachi

⁴Department of Applied Chemistry and Chemical Technology, University of Karachi, Pakistan

⁵Department of Chemical Engineering, NED University of Engineering. & Technology, Karachi, Pakistan

*E-mail: shumailah116@gmail.com

A high performance liquid chromatographic method with UV detection for simultaneous quantification of alprazolam with antihistamine was developed and validated following the ICH guidelines. Separation was achieved on Shimadzu Shim-pack CLC-ODS (M) 25 M column employing mobile phase 80:20methanol-water with pH 3.5 at 230 nm adjusting flow rate 1.0 mL min⁻¹. The linear concentration ranges were 0.2-12.5 µg mL⁻¹ for alprazolam and 0.4-25 µg mL⁻¹ for antihistamines with correlation coefficient greater than 0.998 and detection limits 2.85, 6.92, 10.56, 4.9 ng mL⁻¹ for promethazine, levocetirizine, alprazolam, and loratadine, respectively. Validation showed RSD < 2% and 98.05-101.89% recovery. Proposed method was successfully applied for quantification of studied drugs in pharmaceutical formulations without excipients interference and in human serum.

Keywords: Alprazolam, Antihistamine, Method Validation, HPLC, Pharmaceutical Formulation.



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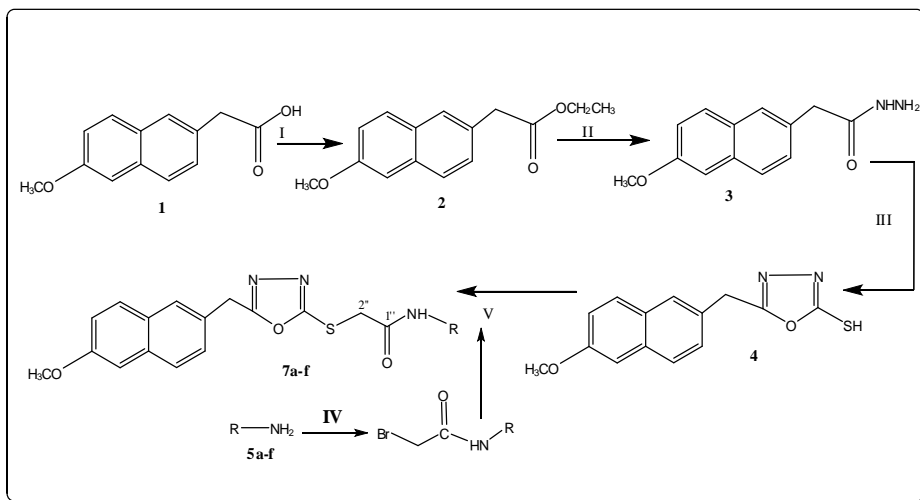
Synthesis and Anti-diabetic Activity of Novel 2,5-isubstituted-1,3,4-oxadiazole Derivatives.

Samreen Gul Khan^{1*}, Kiran Aftab¹, Naheed Akhtar¹

¹Department of Chemistry, GC University, Faisalabad-38000, Pakistan.

*Email: samreengul@gcuf.edu.pk

Oxadiazole is reported to have high synthetic potential for synthesis of many biologically active heterocyclic compounds. Oxadiazole can be helpful in the design of novel highly effective pharmaceuticals with a broad spectrum of bio responses. Oxadiazoles constitute four different classes but 1,3,4-Oxadiazole is the most potent one. The different 2,5-disubstituted-1,3,4-Oxadiazoles possess a large number of biological activities like antifungal, anti-inflammatory and antibacterial [1,2,3]. A series of new *N*-substituted derivatives of naproxen were synthesized in three phases. The first phase involved the sequentially conversion of naproxen acid to ester, hydrazide and 5-benzyl-1,3,4-oxadiazol-2-thiol. In the second phase, *N*-substituted-2-bromoacetamides were prepared by reacting substituted aromatic amines with bromoacetyl bromide in basic media. In the third phase, 5-benzyl-1,3,4-oxadiazol-2-thiol was stirred with *N*-substituted-2-bromoacetamides in the presence of NaH/DMF to get the target compounds. Spectral analysis was used to confirm the structures of synthesized compounds. The synthesized compounds were evaluated for biological activity and were found to have very good anti-diabetic active.



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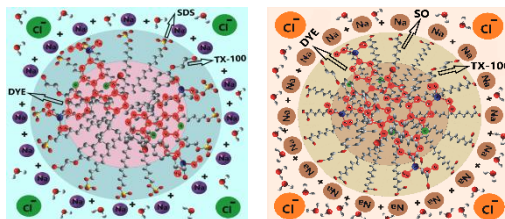
Self-organized Surfactant Assemblies as Nanostructured Dye Carriers: A Mixed Micellar Approach for Enhanced Dye Solubilization as an Application to Remove Dyes from Industrial Effluent by Micellar Enhanced Ultrafiltration

Muhammad Usman^{1*}, Amnah Yusaf¹

¹Department of Chemistry, Govt. College University, Faisalabad, Pakistan

*Email: usm_ca@yahoo.com

Graphical Abstract



The reported work is focused on the solubilization of Rhodamine B (cationic dye), using micellar media of anionic surfactants i.e. Sodium dodecyl sulfate (SDS), Sodium Oleate (SO) as well as mixed micellar media of said anionics with non-ionic surfactant i.e. Triton X-100 (TX-100). The extent of solubilization has been, quantitatively, calculated using data of differential spectroscopy, in term of partition coefficient K_x and Gibbs energy of partition, ΔG_p . It has been observed that mixed micellar media has better solubilization capacity than micellar solution of individual surfactants. Micellar enhanced ultrafiltration (MEUF) has been employed as a potentially attractive tool to remove contaminants from waste water. The dye removal efficiency has been assessed in terms of rejection percentage and permeate flux, using cellulose membrane of 10,000 molecular weight cut off (MWCO). The effects of various factors i.e. ionic strength, concentration of surfactants, concentration of electrolyte, pH, operating pressure and rotations per minute (RPM) has been observed. It has been concluded that the maximum rejection of dye has been observed using micellar media of SDS. Overall, it has been observed that the rejection coefficient of dye is higher at higher concentration of surfactants and electrolyte and at lower values of pH, RPM and transmembrane pressure.

Keywords: Micellar enhanced ultrafiltration, Rhodamine B (RhB), MWCO, Sodium dodecyl sulfate



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Industrial and Agro-Waste Recycling for Mitigating Environmental Pollution and Chemically Analyzed Organic Compost Product

Shaukat Ali Abro^{1*}, Shahida Parveen¹, Aamir Abro², Amjad Ali³, Sana Khokhar⁴, Sameer Ali⁵

^{1,2}Department of Soil chemistry, Sindh Agriculture University Tandojam

²Department of Plant Breeding & genetics, Sindh Agriculture University Tandojam

³Department of Biotechnology, Sindh Agriculture University Tandojam

⁴Department of rural sociology, Faculty of Arts University of Sindh Jamshoro

⁵Department of Livestock management, Sindh Agriculture University Tandojam.

*Email. saabro@sau.edu.pk

Rapid increase in population, industrialization and change in life style and urbanization has resulted in a dramatic increase in industrial and agro wastes. In Sindh there are 34 sugar industries which produce press mud sugarcane is grown 750000 acres. Recycling of this huge waste as compost & other by products has a promising solution. After harvest farmers burn this trash creating carbon fumes wasting a resources & polluting environment. An experiment was conducted for to recycle industrial & agro-waste to produce chemically tested by product as soil amendment. Sugarcane press mud a mill waste and sugarcane trash was co-augulated to make chemically rich organic compost product. The compost was chemically analyzed for parameters like EC, pH, organic carbon, total nitrogen, total phosphorus, total potassium and C/N ratio. The value of EC (3.5), pH (7.3) and C/N ratio 11.63. with highest value of organic carbon (31.80%) was found for Cspm. Result revealed that compost blend was optimum and best, because this blend has rich nutrient concentration of organic matter (54.67%), organic carbon (31.8%), nitrogen (2.73%), potassium (4.6%) and C/N ratio (11.63%) contents. Therefore it is suggested that the industrial and agro-waste could be recycled as compost and subjected to chemical analysis for waste management and reduce soil, water & environmental pollution.

Keywords: Agro-waste recycling, Co-augulated, Press mud,



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II-CC21-P-01



Multivariate Investigation of Toxic and Essential Metals in the Serum of Colorectal Cancer Patients (with Types and Stages) in Comparison with Controls

Muhammad Abdul Qayyum^{1*}, Ahmad Raza Ashraf¹

¹Department of Chemistry, Division of Science & Technology, University of Education Lahore, Pakistan

*E-mail: hmaqayyum@ue.edu.pk

Colorectal cancer (CRC) is currently one of the most frequent malignant neoplasms, ranked 3rd in incidence and 2nd in mortality, both in the USA and across the world. The pathogenesis of CRC is a complex interaction between genetic susceptibility and environmental factors such as exposure to metals. Therefore, the present study was intended to assess the imbalances in the concentrations of selected essential/toxic metals (Pb, Cr, Fe, Zn, Cd, Cu, Se, As, Ni and Hg) in the serum of newly diagnosed colorectal carcinoma patients in comparison with counterpart controls by atomic absorption spectrometry after wet-acid digestion method. Body mass index (BMI) of each study participant and serum carcinoembryonic antigen (CEA) of the CRC patients was determined using immunoradiometric method. Average Ni, Cd, As and Pb levels were significantly higher in the serum of CRC patients compared to the healthy donors; while the average Se, Cu, Fe and Zn concentrations were elevated in controls. The correlation coefficients among the elements in the cancerous patients demonstrated significantly dissimilar communal relationships compared with the healthy subjects. Significant variations in the elemental levels were also showed for various types (primary colorectal lymphoma, adenocarcinoma and gastrointestinal stromal tumor) as well as stages (stage-I, stage-II, stage-III, and stage-IV) among the CRC patients. Majority of the elements revealed perceptible disparities in their levels based on dietary, habitat, gender and smoking habits of the malignant patients and healthy subjects. Multivariate methods revealed noticeably divergent apportionment among the toxic/essential elements in the cancerous patients than the healthy counterparts.

Keywords: Serum; Metals; Colorectal Cancer; Statistical Analysis; Types and Stages



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II-CC21-P-02



Phytochemical and Elemental analysis of Culinary Herbs and Spices

Irfan Ali Mangi^{1*}, Wahid Bux Jatio^{2*}, Fakhar Memon^{1*}

¹University of Karachi, ²Shah Abdul Latif University

*Email: irfanali1414@gmail.com, wahid_jatoi@yahoo.com,
fakhar_memon2@yahoo.com

Plant based natural products are the oldest therapeutic agents throughout the history of mankind. Spices and herbs derived from plants are used in food to produce taste and aroma. These are considered as an essential element in cooking practices of many cultures. Spices and herbs are also rich source of bioactive compounds of medicinal interest known as phytochemicals or secondary metabolites. The phytochemical screening of selected spices demonstrated that most of them contained compounds of great medicinal and dietary values like saponins, flavonoids, steroids, terpenoids, phenolic compounds, cardiac glycosides, anthocyanins, tannins, and carbohydrates. The essential and trace metal concentration was determined by atomic absorption spectroscopy. All samples were rich in amount of Na, K, Ca, Fe, Zn, Cu, Co and Mn that play various vital physiological roles in human health. This study revealed that the use of spices and herbs not only enhance the flavor of the food but also impart the health benefits due to presence of important phytochemicals and essential elements. Present study can be beneficent for food and spices industries and help to develop a combination of spices in such a way that they not only to impart the taste but also nutritional benefits to end users.

Keywords: Phytochemicals, Essential metals, Herbs, Spice



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ICC21-P-03



Antiproliferative Activity of 3, 5-Disubstituted Tetrahydro-2h-1, 3, 5-Thiadiazine Thione (Thtt) Derivatives

Irfanullah^{1,2}, Nuzhat Arshad^{1,3*}, Hamza Azam³, Jamshed Hashim^{1*}, Muhammad Yaseen², Qurat-ul-Ain Hanif^{1,3}

¹HEJ Research Institute of Chemistry, International Centre for Chemical and Biological Sciences (ICCBS), University of Karachi, Pakistan

²Institute of Chemical Sciences, University of Peshawar, Pakistan

³Department of Chemistry, NED University of Engineering Technology, Karachi, Pakistan

*Email: nuzhat@neduet.edu.pk

jamshedhashim@yahoo.co.uk

Four different series of heterocyclic compounds, that is, tetrahydro-2H-1,3,5-thiadiazine thione derivatives were prepared according to the literature¹ and characterized by spectral techniques including ¹H NMR, ¹³C NMR, and Mass Spectroscopy. All derivatives were examined for their antiproliferative activities against two human carcinoma PC3 and HeLa. The toxicity of all the compounds was also determined on normal 3T3 cells. Most of the compounds exhibited significant antiproliferative potential against both cancer cell lines within the range of IC₅₀ = 6.4–29.9 and 2.4–23.8 μM respectively as compared with doxorubicin, as standard. (IC₅₀ = 0.3 μM). The structure–activity relationship indicates that antiproliferative potential depends upon the nature and position of substituents at thiadiazine nucleus. The results indicate that THTT derivatives especially ester derivatives can be a possible prodrugs for the anticancer treatment.

Keywords: Antiproliferative activities, Tetrahydro-2H-1,3,5-thiadiazine thione derivatives

References: Nuzhat Arshad, Jamshed Hashim, Irfanullah, Muhammad Ali Minhas, Javeria Aslam, Tahira Ashraf, Syeda Zehra Hamid, Tahseen Iqbal, Shumaila Javed, **Bioorganic and Medicinal Chemistry Letters**. Vol. 28, No. 19, p. 3251-3254, 2018



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IICC21-P-04



Synthesis of Antiparkinsonian and Antihypertensive Drug Molecule Analogues may Leads to Better Options for Mankind

Sheeba Rizvi¹, Sidra Akhter², Hina Siddiqui², Nasreen Fatima^{1*}

¹Department of chemistry, University of Karachi, Karachi, Pakistan.

²H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan

*Email: nasreenfatima@uok.edu.pk

In the current study, analogues of levodopa and carbidopa had been synthesized to assess their biological activities. Synthesis was carried out by using similar methods in which both were reacted with corresponding alcohols and thionyl chloride in the presence of acetic anhydride. All the synthesized compounds were catecholate. Catechols being oxygen donor ligands, are particularly known of effectiveness for high oxidation state of metals. All the synthesized analogues comprise two free hydroxyl entities that are accessible to chelate metal. Amino and carboxylic group functionalities were blocked by acetylation and esterification process respectively. Ten compounds were documented here on the basis of novelty. A fine crystal of compound 6 was successfully prepared; its XRD analysis shows an orthorhombic structure. Flash chromatography column were used to purify all the synthesized analogues and interpreted by using Mass spectrometry, ¹H NMR, IR and UV-Visible spectroscopy techniques. Characterization was done by NMR which proved the presence of two free catecholic hydroxyl groups. Percentage yield of the compounds was in the range of 33-90%, highest for compound 3 and 6. IR of complexes and ligands showed a drastic change in catecholic region—an evidence of chelation of metal from this site. The verdict is worthy because it was controversial till yet. All synthesized ligands were evaluated for biological activities and found active.

Keywords: Synthesis, Characteristics, Novel compounds, X-ray structure, Biological activity, Chelation



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IICC21-P-05



Comparative Study on Functional Properties of Industrially Important Instant Rice Starch Citrates and Lactates in Mozzarella Cheese

Natasha Abbas Butt^{1*}, TahiraMohsin Ali¹, Abid Hasnain¹

¹Department of Food Science and Technology, University of Karachi, 75270, Pakistan

**E-mail:natashabutt2027@gmail.com*

This present investigation is regarding comparative study of functional properties of extrudates and alcoholic alkaline (AA) treated starches obtained by chemical modification of rice starch citrates and lactates in order to produce instant starches. Mechanical spectra demonstrated that AA is considered a milder treatment compared to extrusion. Drastic increase in functional properties (Swelling power and water binding capacity) occurred after dual modification of pregels. In rheological analysis AA method showed promising values except for % recovery. Thixotropy of extruded starches was significantly less than AA treated starches while SC-20 showed slight time independent behaviour. When applied in imitation cheese both casein replaced (CR) and casein and fat (CR+FR) replaced by extruded starch displayed greater values as compared to AA and control ones which is required for mozzarella cheese. Cross over temperature (T_c) and meltability of extruded starch containing cheese were higher compared to those incorporating AA treated starch lactate. All samples displayed improved cohesiveness and reduced retrogradation tendency after attachment of subsequent functional groups. The extruded starch lactate also formed softer cheese for both CR and (CR+FR) cheese samples. The soft but cohesive cheese samples may allow easy filling of cheese in fried and baked products.

Keywords: Alcoholic-alkaline, Extrusion, Rheology, Thixotropy, Imitation cheese



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IICC21-P-06



Comparative Study on Crosslinked Instant Sorghum Starch Prepared Via Alcoholic Alkaline Treatment and Extrusion Technique

Nusrat Zehra^{1*}, Tahira Mohsin Ali¹, Abid Hasnain¹

¹Department of Food Science and Technology, University of Karachi, 75270, Karachi, Pakistan

*Email: nusrat_zehra@outlook.com

Phosphorus oxychloride (0.1% based on dry starch weight) was used to prepare crosslinked-esterified sorghum starch. Cross-linked starch is permitted as food additives and also allotted E1413 number. Cross-linked sorghum starch (CL) was treated physically by alcoholic alkaline treatment (AAT) and extrusion (EXT) separately. CL-instant sorghum starch excludes the need of heating assembly during processing of many food products. Rheological analysis revealed that both CL-instant sorghum starches exhibited reduced swelling power and pasting viscosity than their native counterparts but stabilized viscosity profile was shown throughout the temperature ramp. Flow curves showed that CL-instant sorghum starches are more resistant to acid, heat and shearing than their native instant starch. For all CL-instant sorghum starches storage modulus (G') was found to be higher than loss modulus (G'') and percent structural recovery of extruded starch was significantly reduced than AAT instant starch. This research aims to explore the effects of crosslinking on instant sorghum starch prepared via AAT and EXT to improve its functionality and increase its utilization in food industries for desired food applications.

Keywords: Sorghum, Instant starch, Crosslinking, Alcoholic alkaline treatment, Extrusion



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IICC21-P-07



Synthesis of Biodegradable Plastics from Wheat Husk

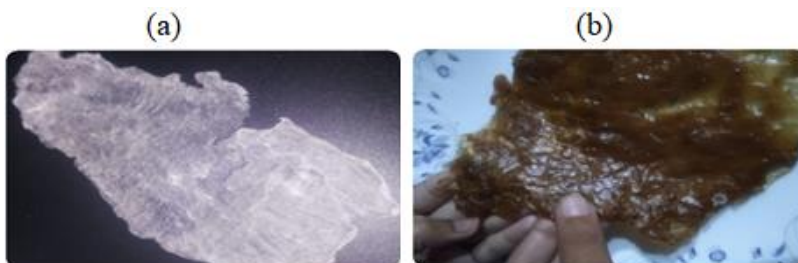
Muhammad Waseem Shahzad^{1*}, Aftab Kareem¹, Zaman Ashraf¹, Ahmad Raza Ashraf¹

¹Department of Chemistry, Division of Science and Technology, University of Education, Lahore, Pakistan

*Email: waseemshahzad0101@gmail.com

Can we live a day without using any plastic products? More than 380 million tonnes of plastics have been produced every year in the world. The pervasive use of plastics demands to assess their potential eco-toxicological impacts. Such concerns can be wiped off, if biodegradable plastic products of same strength and cost be made available. Biodegradable plastics can be synthesized by using the wheat husk and can serve as suitable alternate to polyethylene plastics. The tonnes of wheat husk wasted every year can be made useful in this way. Bioplastics are already available in the market but they are expensive than the conventional plastics. The bioplastics prepared from wheat husk are expected to be cost effective than polyethylene or other counterparts. Most importantly, it would help us breath in pollution free environment. The successful accomplishment of the project would open a new gate for the survival of nature. The preliminary results of the study conducted on developed plastics based on wheat husk, with (Figure a) and without artificial starch (Figure b), showed that their degradation started after 30 days of disposal. Moreover, their strength was also comparable with the polyethylene shopping bags.

Keywords: Synthesis, Biodegradable plastics, Wheat Husk





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IICC21-P-08



Biosynthesis of Lysine in Stirred Fermenter by *Corynebacterium glutamicum*

Saira Bashir^{1*}, Rashida Bashir², Ahmad Adnan¹

¹Department of Chemistry, Govt. College University, Lahore, Pakistan

²Department of Chemistry, University of Education, Lahore, Pakistan

*E-mail: sairabashir@outlook.com

Corynebacterium glutamicum is significant for large scale production of amino acids. The study aims to develop a scheme for production of lysine through fermentation. The microbes were isolated from soil and identified by microscopic examination and biochemical tests. Various carbon sources were tried and molasses was selected as a substrate due to its low-price and abundance. The study provided a cost-effective and well-organized strategy for the production of amino acids. Average biomass yield over a time of 48 hours was 0.337g/g; with a maximum yield within 10 to 20 hours was obtained under optimized conditions: temperature 40°C. The molar yield coefficient of CO₂ was found to be 0.234. The molar yield coefficient of biomass was 0.6 in exponential phase which decreased and fell to near zero at 48 hrs. After 40 hours of fermentation, culture entered into stationary phase, the growth yield turned out to be zero and the total molar yield coefficient of lysine was elevated. Culture conditions of mutants were optimized. Mutants showed optimum lysine production (6.34 g/l) after 48 hours of fermentation at 34°C with pH 7.3, inoculum size 6 % (v/v) and agitation 140 rpm. Optimization of culture conditions significantly improved amino acid production by mutants.

Keywords: *Corynebacterium glutamicum*, Lysine, Fermentation



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IICC21-P-09



Effect of Oxidized Potato Starch as Protein and Fat Replacer in Imitation Mozzarella Cheese

Maria Ahsan^{1*}, Tahira Mohsin Ali¹, Abid Hasnain¹

¹*Department of Food Science and Technology, University of Karachi, Pakistan*

**E-mail: s.maria.ahsan@gmail.com*

Cheese is one of the most famous products around the globe. The world produces cheese with an average market export worth US \$26.7 billion. The rise in the cheese market has also raised prices of cheese. Therefore, different alternates like cheese analogues are introduced in the market. On average 1 kg of cheese substitute is 36% cheaper than 1 kg of natural cheese. Therefore, the present study observed effect of oxidized potato starch in replacing casein, fat and both components in imitation mozzarella cheese. The cheese made with oxidized potato starch showed improved melt and stretch properties as compared to control. The cheese also reduced release of free oil. Whereas, there was no significant difference in the sensory analysis performed. Moreover, rheological analysis of oxidized starch replaced cheese showed that the cheese were softer as compared to control. This trend was also confirmed from textural analysis where reduced hardness, cohesiveness, chewiness, adhesiveness and gumminess were observed. Therefore, it can be concluded that the oxidized potato starch can be successfully used to replace either, casein, fat or both in the imitation mozzarella cheese which would be a potential value added product with cost cutting implication.

Keywords: Potato starch, Oxidation, Imitation Mozzarella cheese



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IICC21-P-10



Kinetic Investigation for the Production of a Significant Antibiotic Bacitracin by *Bacillus licheniformis*

**Rashida Bashir^{1*}, Ahmad Adnan², Ayoub Rashid²,
Quratul Ain³**

¹Division of Science and Technology, University of Education, Lahore

²Department of Chemistry, Government College University, Lahore

³Pakistan Council of Scientific and Industrial Research Laboratories Complex
Lahore, Pakistan.

*E-mail: rashida.bashir@ue.edu.pk

Bacitracin is a potent polypeptide antibiotic used in various combination with other antibiotics for tropical application. Also being a growth ingredient in livestock, it became a very prominent to investigate. The purpose of this study was to evaluate the physical parameters for the optimum microbial production of antibiotic. Study carried out at laboratory scale fermenter under different parameters. Biomass determination carried out by spectrophotometer at 600 nm. Culture tubes (1 cm³) utilized for the quantification of dry biomass in triplet set. Agar Well Diffusion method is used to determine the potency of peptide antibiotic against a test organism *Micrococcus luteus*. The evaluated fermentation media found foremost good for bacitracin activity. Study of kinetics in fermenter revealed that specific growth rate in stirred fermenter was 0.248 for initial twelve hours and 0.157 for shake flask. The number of generation and the generation time found for stirred fermenter were 4.3 and 3.0 h during the exponential growth phase whereas number of generation and generation time for shake flask were 4.05 and 4.4 h. Substrate consumption rate for fermenter and shake flask were 1.617 g/dm³/hour and 1.192 g/dm³/hour for 12 and 18 hours of fermentation, respectively. Another imperative and comparable parameter was specific uptake rate, which was found 0.413 g g⁻¹ h⁻¹ and 0.232 g g⁻¹ h⁻¹ for fermenter and the shake flasks. Combination of effective parameters find out in this study for maximum production of Bacitracin antibiotic at large scale production.

Keywords: *Bacillus licheniformis*, Bacitracin, Specific Uptake Rate, Generation Time, Number of Generation, Kinetic Growth.



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IICC21-P-11



Optimized Enzymatic Glycosylation of Natural *L*-Menthol and Evaluation of Antioxidant Activities of Synthesized Compounds

Shafaq Nisar^{1*}, Muhammad Asif Hanif¹, Muhammad Zahid², Abdul Ghaffar³

¹Nano and Biomaterials Lab, Department of Chemistry, University of Agriculture, Faisalabad, Pakistan

²Department of Chemistry, University of Agriculture, Faisalabad, Pakistan

³Department of Physics, University of Agriculture, Faisalabad, Pakistan

*E-mail: shafaqnisar12@gmail.com

Menthol is a cyclic monoterpene alcohol, present in the *Mentha* leaves, have a number of applications in different products, like candy, toothpastes, vaporubs, confectionary and also in aromatherapy inhalations. However, menthol has low solubility in water. Extensive study has been carried out in order to produce a menthol compound with good water solubility. With this aim, various carbohydrate derivatives of menthol (menthyl glucoside, menthyl maltoside and menthyl fructoside) were synthesized under optimized conditions enzymatically as enzymatic glycosylation of compounds is a valuable tool due to its mildness and selectivity of the conditions of the reactions, compared to chemical methods in which generally harsh reaction conditions or the toxic catalysts use are undesirable. These enzymatic glycosylation methods are considered as good alternative in food additives chemistry where the synthetic chemistry sometimes can't be acceptable. It was found that various factors like, temperature, reactants ratio, enzyme concentration and time have large impact on the yield of synthesized derivatives of menthol. Furthermore, it was observed that among all synthesized carbohydrate derivatives of menthol, menthyl glucoside were have high yield and this compound also showed good antioxidant activities as compare to others.

Keywords: Menthol, Glycosylation, Carbohydrates, Menthyl glucoside, Antioxidant



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IICC21-P-12



Manufacturing of Paver Bricks from Coal Ash: A proposed Methodology for Effective Use of Coal Power Generation Waste

Nukhba Masood^{1*}, Syed Hussain Ali¹, Rabiya Mohammad Iqbal¹, Shahrukh Waseem¹, Sehrish Sarfaraz¹, Mahfooz Soomro³, Suraiya Jabeen², Shagufta Ishteyaque¹

¹Department of Chemical Engineering, University of Karachi, Pakistan

²Institute of Environmental Studies, University of Karachi, 75270, PAKISTAN

³Construction Management, Western Sydney University, Kingswood, Sydney, Australia.

*Email: masoodnukhba@gmail.com

In Pakistan, coal is one of the sources for the generation of low-cost electricity. Pakistan possesses huge coal reserves in Thar region as well as other parts of the country. The use of coal as source of fuel in electric power generation has increased significantly, thus also resulting in the rise in the amounts of waste coal ash from coal power stations every year. Ash produced by these plants can be characterized into two types; bottom ash and fly ash. Generally, in previous years, this waste from power stations ended up in the landfills which could be harmful to the soil and also can contaminate water table below the soil, due to leaching of heavy metals as contained in the ash, by rainwater. Also, Ash can spread in miles around the landfills due to gusty winds, damaging the environment and can force people to leave their adobes and thus create loss to the economy. The main feature of waste management is to avoid the creation of waste by reducing the ash formation and also re-using it by recycling. In Pakistan, the recent advancements include partial substitution of fly ash in the cement manufacturing industry, however, in this paper, the use of fly ash in the manufacture of paver bricks is discussed, which can reduce environmental hazards and can become a beneficial technique to manage waste disposal. This progression in the development of construction materials can be cost effective, environment friendly, and sustainable. This assessment aids in promoting the solution and possible usage of ash in Pakistan.

Keywords: Fly Ash, Waste Management, Environment Friendly.



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IICC21-P-13



g-C₃N₄ Based Tungsten/Molybdenum Oxide Composites: Synthesis, Characterization and Photo Degradation of Organic Pollutants

**Muhammad Tariq^{1*}, Zainab Waheed¹, Muhammad Naeem
Ashiq¹, Naseem Abbas¹, Ajaz Hussain¹, Khalid Mahmood¹**

¹ *Institute of Chemical Sciences, Bahauddin Zakariya University, Multan*

^{*}*E-mail: drtariq2013@hotmail.com*

Photocatalytic degradation of organic pollutant like dyes, from waste water effluents has got attention of scientist because it is one of the applicable and effective methods of get rid of pollutants by using a photocatalyst and sunlight as source of energy. In this study, two g-C₃N₄ based metal oxide ternary composites were synthesized having general formulas g-C₃N₄-WO₃/rGO and g-C₃N₄-MoO₃/rGO by employing facile ultrasonic assisted wet-impregnation methodology. The prepared photocatalysts were characterized by Powder XRD, Scanning Electron Microscopy, Energy Dispersive X-ray studies and Fourier Transform Infrared Spectroscopy. Photocatalytic activity of the synthesized photocatalysts was evaluated by performing photocatalytic degradation test of two different dyes Methylene Blue (MB) and Rhodamine B (Rh-B). g-C₃N₄-MoO₃/rGO shows better degradation efficiency than g-C₃N₄-WO₃/rGO photocatalyst by degrading 79% of Rh-B and 73% of MB in 180 minutes.

Keywords: Photocatalytic, Degradation, Metal Oxide, Composite, Methylene Blue



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IICC21-P-14



Sustainable Pakistani Industries for Lasting Future

Sajid Ali¹, Aresha Ali Khan¹, Rajkumar Dewani^{2*}, Abdur Raheem¹, Omer, Kehkashan Khan¹, Muhammad Ali Versiani¹

¹*Department of Chemistry, Federal Urdu University of Arts Science & Technology, Karachi-75300, Pakistan*

²*Pakistan Council of Scientific and Industrial Research (PCSIR) Leather Research Centre (LRC), Karachi, Pakistan*

**E-mail: rajdewaan@gmail.com*

Pakistan is an Agro-industrial state striving to establish its place in the global economy. The need of the hour for industrialized nations is the drive towards sustainability. Sustainability in the world of technology stands on the twelve pillars of Green Chemistry. This study sheds light on the possibility for our process industries to upgrade in order to be more sustainable on grounds of environment, economy, safety and international recognition. The recommendations have been put forward considering the type of industries in Pakistan, their current state, case study reports and the possible applications of core Green Chemistry Principles. The highlighted areas include industrial interlinks for material exchange, adaptation to renewable feedstock's, process optimizations with reference to monitoring, energy efficiency, better yields and less waste generation etc. Suggested pathways could open new doors for economic growth, international trade benefits and would improve the global image of Pakistan towards a lasting future.

Keywords: Green Chemistry, Sustainability, Biofuel, Biopolymers, Industrial Linkage



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IICC21-P-15



Development of Organic Skincare and Natural Cosmetics: A New Startup (Business + Chemistry) for Local Industry

Sana Wahid^{1*}, Samiyah Tasleem¹, Sajid Jahangir¹, Urooj Haroon¹, Sana Nazeer¹

¹*Department of Chemistry, Federal Urdu University of Arts, Science & Technology, Karachi, Pakistan*

**Email: sanawahid90@gmail.com*

Caring for our skin is one of the easiest ways to ensure long term skin health and radiance. Natural cosmetics development is a progressive startup to provide you with a balance in the skincare and body products you use daily. Unfortunately, many personal care products in the market today, even natural skincare lines, contain hormone-disrupting xenoestrogens. Our main goal is to merge the idea of natural organic skincare products with pharmaceutical standards using nature's own pure ingredients. Organic skincare products are great fun to make as they combine essential vitamins, botanicals, and minerals that heal and restore our skin without harming earth. The development of natural skin care brands are dedicated to redefining beauty industry standards for products that are not only good for us but also good for our planet. At present, we have developed organic soap using different oil blends and herbs. Our organic natural soap recipes are meticulously developed to produce a mild skin nourishing soap that offers a magnificent long lasting lather and leaves your skin feeling clean, soft and radiantly healthy.

Keywords: Organic Skin Care, Natural Cosmetics, Soaps, Botanicals



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IICC21-P-16



Labeling and Biodistribution of ^{99m}Tc - Fludarabine for Medical Purposes

**Tanveer Hussain Bokhari^{1*}, Sara¹, Muhammad Khalid²,
Muhammad Nadeem Lodhai², Muhammad Usman¹**

¹Department of Chemistry, Government College University, Faisalabad,

²Isotope Production Division, Pakistan Institute of Nuclear Science and
Technology, Islamabad, Pakistan

*E-mail: tanveer.bokhari@yahoo.com

Fludarabine is a chemotherapeutic agent used to treat different types of lymphoma and leukemia. Technetium-99m is most widely used radiotracer in radiopharmacy centers worldwide. The objective of this work was to demonstrate direct radiolabeling of fludarabine phosphate with Tc-99m for diagnostic purposes. The optimizations carried out for this purpose involved variations in the amount of ligand (100-900 μg), quantity of $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ (10-100 μg), pH range 3-11 using 0.1 N NaOH and 0.1 N HCl. Biodistribution was performed in balb-c mice at different time points. The optimum conditions that experienced the highest radiolabeling efficiency (98 %) were included with 500 μg fludarabine, 30 μg stannous chloride, pH 8.5 with 3-4 mCi TcO_4 incubated for 30 minutes at room temperature. The biodistribution of ^{99m}Tc -Fludarabine was also performed in mice.

Keywords: Fludarabine, Chemotherapeutic Agent, Radiopharmacy Centers



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IICC21-P-17



Analysis of Water Quality Index of River Yamuna at Allahabad Region

Runit Isaac^{1*}, Prerna Higgins¹

¹Department of Chemistry, Sam Higginbottom University of Agriculture
Technology and Sciences, Prayagraj, U.P. India

*Email: shalome.runit@gmail.com

Yamuna River is considered as one of the most sacred river in India. Many industrial waste and household sewage water are directly discharge into river without treatment, thus making the water body polluted. The aim of this study is to analyse the water quality parameters of Yamuna River at three locations in pre and post winters in Prayagraj city, and development of water quality index using thirteen parameters pH, Total Dissolved Solids (TDS), Turbidity, Hardness, Biological Oxygen Demand (BOD), Dissolved Oxygen (DO), Chemical Oxygen Demand (COD), Mg^{2+} , Ca^{2+} , Iron, Alkalinity, Cl^- , and SO_4^{2-} which were analyzed by standard procedures of APHA. The values obtained were compared with the guideline values for drinking water by Bureau of Indian Standard (BIS) and World Health Organization (WHO). All the samples were collected in 2 liters of polyethylene bottles pre cleansed by distilled water and well dried. The methods used include titration, and gravimetry as per the standard methodology proposed by the American Public Health Association, 2007. The analyzed data were compared to the WHO recommended standards and further calculated to evaluate the relationship between different parameters of the collected samples. Water Quality Index (WQI) is an important statistical tool for determination of the drinking water quality in rural, urban and industrial regions. It reflects the composite influence of different water quality parameters. The WQI of Yamuna river water was calculated for three locations. It was observed that WQI values ranges from 50 to 100 which falls in the range of good quality of water. It is shown that WQI may be a useful tool for assessing water quality and predicting trend of variation in water quality at different locations in the Yamuna River.

Keywords: Water Quality Index, Yamuna River, Water Quality Parameters



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IICC21-P-18



Reduction of Cr(VI) from Tannery Effluent by ZnO/CuO Composite

**Nida Naeem¹, Ijaz Ahmad Bhatti¹, Ambreen Ashar¹,
Muhammad Mohsin¹**

¹Department of Chemistry, University of Agriculture Faisalabad,

*E-mail: nidanaeem77@gmail.com

Efficient reduction of toxic heavy metals such as Cr(VI) by heterogeneous photocatalysis based on metal oxide has become attention of research due to their harmful influence on environment. Here, pure ZnO, pure CuO nanoparticles and their composite was synthesized by microwave-assisted sol gel method. Fabrication of ZnO/CuO@bark was done by dip-coating method and their photocatalytic activity towards the reduction of hexavalent chromium under the exposure of solar light was studied. When synthesized material was characterized by (XRD), (SEM), (EDX) and (FT-IR) results showed the hexagonal-monoclinic morphology, having crystallite size 23 nm, spherical shape, high chemical purity and functional group confirmation, respectively. Hexavalent chromium reduction in tannery effluent was determined by employing UV-vis spectroscopy, AAS and Raman spectroscopy. Process parameters such as pH, sunlight irradiation time and initial concentration of heavy metal were optimized by using RSM. The optimized conditions such as pH: 7, sunlight irradiation time: 3 hours and initial concentration of heavy metal: 30 ppm were proved and 92% reduction of Cr(VI) was almost achieved under these conditions. Fabricated photocatalyst such as ZnO/CuO@bark indicated excellent reusability and 50% activity was decreased greatly. The results demonstrated that ZnO/CuO@bark have remarkable potential for the remediation of toxic heavy metals present in tannery effluent.

Keywords: Photocatalysis, Advanced Oxidation Processes (Aops), Hexavalent Chromium, Semiconductor Metal Oxide, Tannery Effluent



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IICC21-P-19



Synthesis and Applications of Silver Nanoparticles of *Buxus wallichiana*

Noor Ul Ain¹, Wajheeba Khan¹, Nargis Jamila^{1*}

¹Department of Chemistry, Shaheed Benazir Bhutto Women University,
Peshawar, Khyber Pakhtunkhwa, Pakistan

*Email: nargisjamila@sbbwu.edu.pk

Buxus wallichiana commonly known as Himalayan boxwood belongs to family Buxaceae. It is an evergreen shrub and can be found at high, shady, and cold places growing to height of six meters. Traditionally, it is used as bitter tonic, analgesic, antiseptic, in hemorrhoids, and as a growth stimulant especially in hair growth. This study reports the synthesis of *B. wallichiana* aqueous extract silver nanoparticles (BWAgnPs) and the redox catalytic activity of. From the results of BWAgnPs synthesized in a ratio of 1:1 to 1:25, under stirring, heating and stirring, incubation, and sunlight, it was found that under sunlight in the ratio of 1:25 (extract:salt), significant and well stable nanoparticles were formed as depicted from the sharp intense UV absorption peaks. The synthesized BWAgnPs tested against several dyes including methyl orange, congo red, methylene blue, ortho-nitrophenol, and para-nitrophenol showed potent redox catalytic activity in the degradation of the subject dyes. This study conclude that the subject AgNPs can be used in the removal of organic pollutants from wastewater.

Keywords: *Buxus wallichiana*, Silvernanoparticles, Sunlight, Dyes



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IICC21-P-20



Synthesis, Characterization and Applications of Gold Nanoparticles of *Polygonum afghanicum*

Malka Saba¹, Faryal Khan¹, Nargis Jamila^{1*}

*1Department of Chemistry, Shaheed Benazir Bhutto Women University,
Peshawar, Khyber Pakhtunkhwa, Pakistan*

**Email: nargisjamila@sbbwu.edu.pk*

Polygonum afghanicum belongs to Family and is a rich source of phenyl propanoids, acetophenones, chalcones, coumarins, flavonoids, lignans, naphthoquinones, anthraquinones, sesquiterpenoids, triterpenoids, stilbenoids and tannins. The study research work describes the synthesis of gold nanoparticles, antioxidants and catalytic properties of *P. afghanicum* natural ethanolic extract (PAAuNPs). The results of AuNPs synthesis showed that the ethanolic extract yielded significant amount of AuNPs using 1:5 ratio of natural ethanolic extract and gold salt solution in the sunlight. The synthesized AuNPs showed enhanced antioxidant and redox catalytic potential in the dyes degradation.

Keywords: *Polygonum afghanicum*, Sunlight, Gold nanoparticles, Dyes, Antioxidant



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IICC21-P-21



Green Synthesis of Silver Nanoparticles using *Chenopodium botrys* (Jerusalem oak)

Malka Saba¹, Nargis Jamila^{1*}

¹Department of Chemistry, Shaheed Benazir Bhutto Women University,
Peshawar 25000, Khyber Pakhtunkhwa, Pakistan

*Email: nargisjamila@sbbwu.edu.pk

Green association of metallic nanoparticles has been gotten to oblige diverse natural materials (e.g., microorganisms, parasites, green development, and plant isolates). We investigated that *C. botrys* is well known for its applications in the treatment of different sicknesses like pectoral grumblings, cough, stomach torment, pneumonic check and in apprehensive warm gestures. The herb contains alkaloids, flavonoids and several terpenoids, which exhibit several significant therapeutic potential for growing new drugs. The current study reports the synthesis of silver nanoparticles (CBAgNPs) and their antioxidant and catalytic properties synthesized using *C. botrys* aqueous extract in different ratios under sunlight, stirring, stirring and heating, and incubation. From the results, it was found that the production of CBAgNPs was significant using 1:0 ratio, 1:15 ratio of aqueous extracts and AgNO₃ salt solutions, respectively. The synthesized AgNPs demonstrated potential antioxidant and catalytic activities.

Keywords: *Chenopodium Botrys*, Stirring, Silver Nanoparticles, Dyes, Antioxidants



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IICC21-P-22



Plant-mediated Green Synthesis and Biological Activities of Polysaccharide Nanoparticles through Top-Down Approach

Asif Ahmad¹, Behramand^{1*}

¹Islamia College University, Peshawar, Pakistan

*E-mail: dr.bhramand@icp.edu.pk

Hot-water extraction of polysaccharides of different polarities namely PS-60, PS-70, and PS-80 from medicinal plant *Rosa webbiana*, the formation of their nanoparticles, and evaluation of their biological activities are described. The crude polysaccharides were deproteinized using a combination of the HCl and CaCl₂ methods. The vibrational spectrum showed H-bonded hydroxyl stretching (3250 cm⁻¹), sp³C-H stretching (2920 cm⁻¹), COO⁻ group stretching (1610 cm⁻¹), –CH₂– bending (1440 cm⁻¹), C-C stretching (1233 cm⁻¹), and C-O-C etherial group (1020 cm⁻¹) stretching bands characteristic of polysaccharides. The small chain polysaccharides were shown superior radical scavenging, anti-bacterial, anti-fungal and anti-leishmanial properties than the medium and long-chain polymers. SEM studies of nanoparticles were shown well distributed and smooth spherical nanoparticles with an average size of 14 nm. Both polysaccharides and their nanoparticles were shown excellent bactericidal properties against *S. typhi*, *E. coli*, and *P. argenusa* and *Enterococcus facelisis* superior to the standard ceftriaxone. The nanoparticles strongly inhibited the growth of *Rhizophus* and *Trichoderma* at high concentrations and inhibited the growth of *Acromonium* at low concentrations. Both the polysaccharides and nanoparticles were also found to show moderate to high anti-leishmanial properties at concentrations as low as 25 µg/mL.

Keywords: *Rosa webbiana*, Nanoparticles, Polysaccharides, *P. argenusa*, *Rhizophus*



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IICC21-P-23



Synthesis and Characterization of Sweet Potato Starch Based Composite Bioplastic by Incorporation of ZnO Nanoparticles

Saira Iqbal¹, Arjumand Iqbal Durrani¹, Ashi Rashid¹

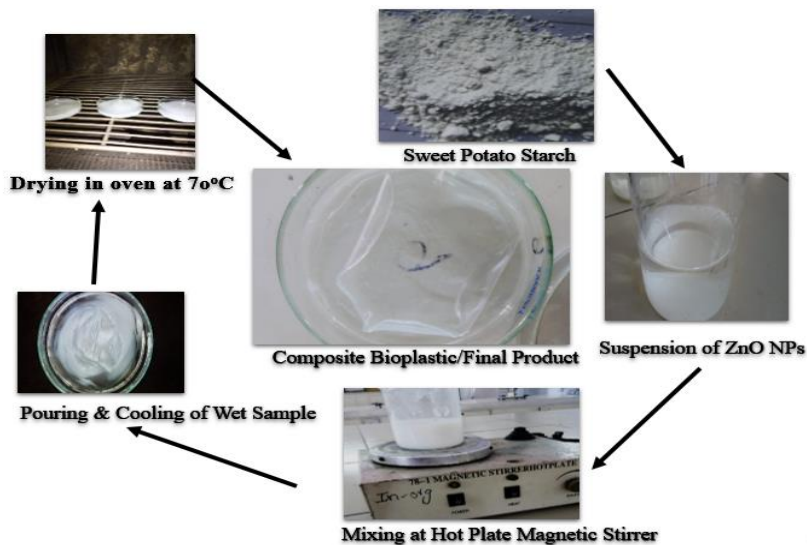
¹Department of Chemistry, University of Engineering, & Technology, Lahore

*E-mail: sairaiqbal900@gmail.com

The shocking rate of environmental toxic waste produced by single-use plastics has compelled the quest for evolving sustainable yet, cost-effective alternatives. This study intended to develop bioplastic films from renewable energy sources. The composite bioplastics were developed using sweet potato starch by incorporation of biogenically synthesized ZnO nanoparticles to avoid any harmful side products. TGA, DSC, SEM, FT-IR, and UV-Visible spectroscopy analysis were performed to characterize the morphological, chemical, and thermal parameters of bio nanocomposite. FT-IR spectra demonstrated that the shift in the peaks confirms relation between the polymer matrix and the ZnO NPs. Maximum UV absorption and transparency were displayed by the bioplastic film reinforced by ZnO NPs. In thermogravimetric analysis (TGA), steady decrease occurring between 240 °C to 410 °C indicate thermal decomposition of bio nanocomposite at 339.60 °C. Differential scanning calorimetry (DSC) test revealed high melting temperature (T_m) of 144°C for starch film and 201.86 °C for bio nanocomposite. The results from SEM analysis exhibited enhanced morphologies in bio nanocomposite films for its fewer spaces and cracks. Biodegradability of bio nanocomposite films was determined through soil burial method. Bioplastic developed in this study can be an alternate to the prevailing conventional plastic with potential use in packaging industry.

Keywords: Bioplastic, Nanoparticles, Biogenically, Bio nanocomposite, Biodegradability

Graphical Abstract:



Highlights:

- Biodegradable Plastic as Sustainable Packaging Material
- Use of Biogenecally Synthesized ZnO NPs as Fillers
- Enhanced Thermal Properties of Bioplastic Films



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IICC21-P-24



Photocatalytic Degradation of Textile Wastewater Using Immobilized CuCo_2O_4 Nanocomposite Thin Films

Muhammad Mohsin^{1*}, Ijaz Ahmad Bhatti¹, Muhammad Fuqran¹, Ambreen Ashar^{1,2}

¹Department of Chemistry, University of Agriculture, Faisalabad,

²Department of Chemistry, Government College Women University, Faisalabad

*E-mail: m.mohsin618@gmail.com

Up to 84000 tons of dye can be lost in water, and 90 million tons of water are attributed annually to dye production and their application. The industrial wastewater has become a leading source of water pollution due to diverse nature of pollutants present in the effluents which are hazardous and toxic. Present study was focused on the fabrication of CuCo_2O_4 nanocomposite thin film over metal beads at 500 °C by spray pyrolysis method, fabricated material was characterized by XRD, FTIR, SEM, Zeta potential. The independent variables such as irradiation time, pH, concentration of H_2O_2 and concentration of dye RB were optimized using response surface methodology for maximum degradation of pollutant. The photocatalytic degradation efficiency of immobilized CuCo_2O_4 nanocomposite thin film was evaluated by studying degradation and mineralization of dye RhB. Maximum photocatalytic degradation (94%) of RhB dye was achieved at optimum condition (pH: 7, sunlight irradiation 3hrs., oxidant concentration: 30 ppm and initial dye concentration: 30 ppm). Effective degradation of RhB dye was confirmed by UV Vis-spectroscopy and High-performance liquid chromatography. After treatment % reduction in COD, BOD, TOC, pH, EC, TDS and reusability of photocatalyst was also evaluated.

Keywords: Wastewater Treatment, Nanocomposites, RSM, HPLC, Water Quality Parameters



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IICC21-P-25



***Forsskaolea tenacissima* Root Mediated Silver Nanoparticles and their Catalytic Properties in Dyes Degradation**

Wajheeba Khan¹, Noor Ul Ain¹, Nargis Jamila^{1*}

¹Department of Chemistry, Shaheed Benazir Bhutto Women University,
Peshawar, Khyber Pakhtunkhwa, Pakistan

*Email: nargisjamila@sbbwu.edu.pk

Forsskaolea tenacissima (Nettle Desert) belongs to the family Urticaceae is comprised of six species distributed throughout the world including Pakistan. It is traditionally used in wound healing and hemostatic in many countries. Its herbal tea known as tisane is used to treat rheumatoid arthritis and for the removal of bile stone. It has been reported to have anti-inflammatory, antispasmodic, antidiabetic, and antipyretic activities. Keeping in view the medicinal importance of *F. tenacissima*, the present research work was carried out to synthesize their silver nanoparticles (FTRAgNPs) under different conditions of stirring, heating and stirring, incubation, and sunlight in different ratios (1:1 to 1:20). The results showed that the most stable nanoparticles were formed under the condition of sunlight in 1:9 and 1:19 ratios. The synthesized nanoparticles evaluated for catalytic activity in dyes degradation showed that they could significantly reduce methyl orange, congo red, methylene blue, ortho-nitrophenol, and para-nitrophenol. Hence, the subject AgNPs could help in organic pollutant removal.

Keywords: *Forsskaolea tenacissima*, AgNPs, Sunlight, Catalytic Activity



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IICC21-P-26



Synthesis of Ag Nanoparticles using *Lespedeza juncea* and their Application as Environmental Remediation Agent

Hafiza Salma Bibi¹, Sana Ihsan¹, Nargis Jamila^{1*}

¹Department of Chemistry, Shaheed Benazir Bhutto Women University,
Peshawar, Khyber Pakhtunkhwa, Pakistan

*Email: nargisjamila@sbbwu.edu.pk

Lespedeza juncea belongs to family Fabaceae/Leguminasae is widely distributed in the hilly areas of Pakistan including Swat, Kurram agency, Orakzai agency, and Kashmir. It is a rich source of flavonoids, protochechuic acid, catechin, and alkaloids and is traditionally used as anthelmintic, depurative, and tonic. Its decoction is used in tuberculosis, hernia, dental caries, snakes and dog bites, ulcer, and dysentery. The present research work describes the synthesis of silver nanoparticles (LJAgNPs) utilizing its aqueous extract and silver salt in different ratios (1:5 to 1:25). In addition, the catalytic activity of the synthesized LJAgNPs was evaluated in dyes degradation. The results of AgNPs synthesis showed that the prominent and stable AgNPs were formed in 1:25 ratio under hearing and stirring condition. The synthesized nanoparticles were found very efficient catalytic agent in dyes; methyl orange, methylene blue, para-nitrophenol, ortho-nitrophenol, and congo red, which suggests its application in the removal of dyes pollutants from wastewater.

Keywords: *Lespedeza juncea*, silver nanoparticles, heating and stirring, methylene blue.



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Synthesis of *Ocimum americanum* Silver Nanoparticles and their Catalytic Activity Dyes Degradation

Zainab Mushtaq¹, Nargis Jamila^{1*}

¹Department of Chemistry, Shaheed Benazir Bhutto Women University,
Peshawar 25000, Khyber Pakhtunkhwa, Pakistan

*Email: nargisjamila@sbbwu.edu.pk

Ocimum americanum (sweet basil) belongs to family Lamiaceae is an annual herb with white or lavender flowers. Different part's extracts of *O. americanum* possessing antioxidants, antidysentric, antidiabetic, and antimicrobial properties. The current study is conducted on the synthesis of silver nanoparticles of its aqueous extract (OA-AgNPs) in different ratios of 1:9 to 1:17 under sunlight, stirring, heating and stirring, and incubation. The results revealed that under sunlight in the ratio of 1:9 significant amount of OA-AgNPs were formed represented from the sharp intense UV absorption peaks. The synthesized OA-AgNPs evaluated for catalytic property in dyes degradation including methyl orange, congo red, methylene blue, *ortho*-nitrophenol, and *para*-nitrophenol showed significant redox catalytic activity. The study concludes that the subject AgNPs can be used in the removal of organic pollutants from wastewater specially textile wastewater.

Keywords: *Ocimum americanum*, Silver Nanoparticles, Sunlight, Methyl Orange



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Synthesis of Nickel Copper Zinc Ferrate Nanocomposites for the Cost Effective Statistically Optimized Rapid Decontamination of Organic Pollutant from Wastewater

Sana Sheikh^{1*}, Muhammad Saad^{1*}, Hafsa Wahid¹

¹Department of Chemistry, University of Karachi, Pakistan

*E-mail: sid99@gmail.com, saad@uok.edu.pk

The current research focuses on the green synthesis of nickel copper zinc ferrate nanocomposites by co-precipitation method. The nanocomposites were characterized by Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray spectroscopy, and Fourier Transformed Infrared Spectroscopy (FTIR). The surface charge was determined by pH_{pzc} . The nanocomposites were employed as high-performance adsorbent for the decontamination of turquoise blue. The adsorption experiment was optimized by Response Surface Methodology (RSM) based on Central Composite Design (CCD) that predicted a removal of 98.83% under optimum conditions. Replicate 5 runs affirmed the optimum parameters with %RSD and % Mean Error of 0.6563% and 2.406% respectively. Significance of model and individual parameters was assessed by ANOVA and pareto analysis. Among various models, Freundlich and pseudo first order models were the best fit isotherm and kinetic models respectively as affirmed by error analyses. Spontaneity of the adsorption process was affirmed by thermodynamic studies. Conclusively, the proposed method is an ecofriendly and rapid method for the environmental remediation purpose.

Keywords: Adsorption, Central Composite Design, Desorption, Nanocomposites, Purification, Response Surface Methodology, Salt Effect, Wastewater Treatment.



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Characterization of the CNT-Hematite Nano-hybride Synthesized by Wet Chemical Method

Danish Raza^{1*}, Syed Farhan Hasany²

¹ *Department of Physics, NED University of Engineering & Technology,
Karachi, Pakistan.*

² *Department of Chemistry, NED University of Engineering & Technology,
Karachi, Pakistan.*

**Email.danishraaza@yahoo.com*

This work concerned with the Nano-hybrids (NHs) which shows the unique and enhanced physicochemical properties depending upon their size, structure and composition in comparison to a single pre-synthesized components of NHs. The nanohybrid (NPs) of Carbon-Nano-Tubes (CNT) conjugated with iron oxide nanoparticles (NPs) were prepared by wet chemical method. The Synthesized nanoproduct was investigated by X-ray diffraction (XRD), Scanning electron microscope (SEM). Fourier Infrared Transform Spectroscopy (FTIR), Vibrating sample magnetometer (VSM) to determine size, shape, structure, composition and magnetic properties of the synthesized material. It implies that the chemical wet method is simple, reproducible, cheap and that's why a promising route to decorate many other materials on the CNT. Structural morphological and magnetic Investigation of the composite reveals that it is a suitable material for the lithium-ion batteries and/or the supercapacitors. Therefore, Future research must be carried out to be implement the nanocomposite in other applications.

Keywords: Nanohydride, Nanocomposite, Wet Chemical Method



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Designing Self-healing Nanocomposite Hydrogels of Biopolymer with Metal Nanoparticles by Green Chemistry Approach as Future Injectable Anticancer Materials

Musammir Khan¹

¹University of Wah, Pakistan.

Email: musammir.khan@uow.edu.pk

Recently, the biopolymer based self-healing hydrogels are ideal candidate for the fabrication of injectable drug delivery systems. The nanocomposite hydrogels obtained from the renewable biobased resources by green chemistry approach were investigated here as therapeutically important future anticancer agent. The water soluble chitosan (WSC) was obtained by grafting biocompatible glutamic acid onto the chitosan chain. This WSC showed fast gelation ($t \approx < 60$ s) with benzaldehyde terminated 4-arm/branch polyethylene glycol as crosslinker. The compression modulus of these hydrogels was dependent on both the crosslinker content as well as total solid content in the final gel and can be controlled between 5-67 kPa. Moreover, the gel showed injectability and complete self-healing ability at the lower solid content (2 %). The antioxidant, gallic acid capped metallic (silver-Ag and gold-Au) nanoparticles (NPs) was synthesized and used for the fabrication of nanocomposite hydrogels. These nanocomposite hydrogels showed good biocompatibility as tested against normal fibroblast cell line. The anticancer activity was investigated using lung cancer cell line for 24 h and 3 days, which showed that only the composite hydrogels incorporated with AuNPs was effective against cancer cell apoptosis in comparison to all other nanocomposites and blank gels. Therefore, this study opens a new opportunity to use nanocomposite hydrogel materials as an effective alternative to beat cancer in the future.

Keywords: biopolymer, self-healing, antioxidant, metallic nanoparticles, composite hydrogel, anticancer



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Designing of Reusable Amine-Functionalized Zerovalent Bimetallic Magnetic Nanoparticles for Efficient Sequestration of Azo dyes From Water: Kinetics & Thermodynamics Studies

Abira Saleem¹, Qurrat ul Ain^{1*}, Hina Anwar¹, Muhammad Raza Shah²

¹ Department of Chemistry, University of Karachi, Pakistan

² H.E.J. Research Institute of Chemistry, ICCBS, University of Karachi, Pakistan

*E-mail: qurrat_chem@uok.edu.pk

The Fe/Ni bimetallic nanoparticles (BNPs) are of substantial current concern with splendid applications in environmental remediation, biomedicine, hydrogen storage, etc., due to their high surface area, corrosion stability and magnetism, while low thermal expansion, toxicity and cost. The present study was aimed to synthesize biocompatible amine-functionalized Fe/Ni-BNPs (AM-Fe/Ni-BNPs) to remove precarious (carcinogenic, mutagenic) industrial azo dyes from water by batch adsorption. The structure of AM-Fe/Ni-BNPs was affirmed by several techniques: FT-IR spectroscopy, AFM, SEM-EDS, TGA, pH_{zpc}, etc. Acid Red 27 (AR27) removal was optimized through study of effect of various experimental parameters on removal efficiency. AM-Fe/Ni-BNPs removed AR27 upto 99.7% (from deionized water) and 89.2–99.3% (from drinking/tap water) within 60 minutes at pH 4, 25°C, 12 mg/L dye and 0.5 g/L adsorbent. The salt decreased the AR27 removal; however, the effect at lower salt concentration was negligible. The adsorption data were fitted well to Langmuir isotherm (q_{max} = 133.3 mg/g) and pseudo-second-order-kinetics model with film diffusion as a dominant mechanism. Thermodynamics indicated spontaneous, exothermic adsorption process. Furthermore, AM-Fe/Ni-BNPs easily desorbed in alkaline medium and showed excellent reusability. This study builds up AM-Fe/Ni-BNPs as a proficient, green and economic tool to eliminate harmful colored contaminants from the real industrial effluents in future.

Keywords: Iron/Nickel NPs, Chemical Reduction, Morphology, Adsorption, Equilibrium, Regeneration



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IICC21-P-32



Synthesis of Copper Nanoparticles for the Cost Effective Statistically Optimized Rapid Removal of Dye by Adsorption Method

Misbah Saleem^{1*}, Muhammad Saad^{1*}

¹Department of Chemistry, University of Karachi, Pakistan

*E-mail: misbahhchemist98@gmail.com, saad@uok.edu.pk,

The current research focuses on the synthesis of copper nanoparticles by co-precipitation method. The nanoparticles were characterized by Scanning Electron Microscope (SEM), Energy Dispersive X-Ray Spectroscopy (EDS), Fourier Transformed Infrared Spectroscopy (FTIR). The surface charge was determined by pH_{pzc} . The nanoparticles were employed as high-performance adsorbent for the decontamination of Reactive Navy Blue dye. The adsorption experiment was optimized by Response Surface Methodology (RSM) based on Central Composite Design (CCD) that predicted a removal of 99.79% under optimum conditions. Replicate 6 runs affirmed the optimum parameters with %RSD and % Mean Error of 0.0652 and 0.1441 respectively. Significance of model and individual parameters was assessed by ANOVA and pareto analysis. Among various models, Freundlich and pseudo second order models were the best fit isotherm and kinetic models respectively as affirmed by error analyses. Spontaneity of the adsorption process was affirmed by thermodynamic studies. Conclusively, the proposed method is an ecofriendly and less expensive method for the environmental remediation purpose.

Keywords: Adsorption, Central Composite Design, Nanoparticles, Purification Cost Analysis, Response Surface Methodology



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One Pot Ultrasonic Green Synthesis of Carbon Dots and their Application in Visible Light Induced Dye Photocatalytic Studies

**Maria Zaib^{1*}, Amna Arshad¹, Saira Khalid¹,
Tayyaba Shahzadi¹**

¹*Department of Chemistry, Faculty of Physical Sciences, Government College Women University, Sialkot, 51310, Pakistan*

**E-mail: maria.zaibl@gcwus.edu.pk*

A simple, environment friendly and cost-effective approach to prepare carbon dots is reported in this study. Leaves of *Polyalthia longifolia* were utilized as carbon source to synthesize carbon dots by ultrasonication. These are then characterized by UV-visible, Fourier transform infrared, X-ray and Ramanspectroscopy. UV-visible spectrum of prepared carbon dots exhibited two absorption peaks at 225 and 260 nm. Fourier transform spectrum of carbon dots exhibited the different functional groups at absorption peak values of 1650 cm^{-1} , 2989 cm^{-1} , 1471 cm^{-1} , 1762 cm^{-1} and 1126 cm^{-1} , respectively. X-ray diffraction analysis of carbon dots showed the amorphous nature of carbon dots with peak values at 31.38° and 40.93° respectively. Raman spectrum of synthesized carbon dots showed two absorption peaks at 541 and 741 nm. These prepared carbon dots were further used for photocatalytic removal of congo red dye and methylene blue dye. The maximum removal of methylene blue dye was achieved at pH 8, at a dye concentration of 5 mg/L in a time interval of 60 minutes. In case of congo red dye, maximum degradation was observed in acidic medium at a pH of 6 with 5 mg/L dye concentration in a time interval of 90 minutes.

Keywords: Carbon dots; green synthesis; photocatalysis; methylene blue dye; congo red dye



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PANI/HNT Based Nano-Composite as an Efficient Adsorbent for the Removal of Diclofenac Sodium from its Aqueous Solution

Prerna Higgins^{1*}, Shaziya H. Siddiqui¹, Runit Isaac¹

¹*Department of Chemistry, Sam Higginbottom University of Agriculture Technology and Sciences, Uttar Pradesh, India.*

**E-mail: prehig@yahoo.in*

Survival without water is not doable as water and any sort of contamination in water prior to living beings will have a baleful effect on the environment. Pharmaceutical pollution in water is an influential aspect which has raised substantial environmental concern. The wastewater treatment plants are possessing struggle to treat these recalcitrant contaminant completely to its eradication. A relentless approach is a necessity in order to remove contaminants from water. Therefore the present study focuses of removing Diclofenac sodium employing PANI/HNT. The maximum removal of diclofenac sodium using PANI/HNT was obtained at pH 3.0 and at 60 min equilibrium time. The maximum adsorption capacity of drug was found to be 179.94 mg/g. The kinetic data was best fitted in Pseudo 2nd order kinetic model and Freundlich was the best suited adsorption isotherm.

Keywords: Pharmaceutical, Diclofenac, Removal, Adsorption, Freundlich, Kinetics.



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Synthesis of Antimicrobial Peptide and its Anticancer Activities

Serab Khan¹, Farzana Shaheen^{1*}

¹H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan.

*E-mail: afnan.iccs@gmail.com

The antimicrobial peptide, temporin-LK1, which includes 17 residues, reported to have strong antimicrobial activities against some fungi, Gram-positive and Gram-negative bacterias. It was isolated from the skin secretion of frog, *Limnonectes kuhlii* (Ranidae) and its structure was elucidated by HR/EI-MS, NMR and MALDI-TOF/TOF. The antimicrobial activities of temporin LK1 and its analogs has recently reported by our research group against drug resistant strains of *S. aureus*. In current study, we have synthesized natural product temporin-LK1 and its analogs to study their anticancer activity against different cancer cell lines. The natural product was found to be highly active against MCF-7 cell line.

Keywords:Antimicrobial peptide, temporin-LK1, *Limnonectes kuhlii*, *S. aureus*, MCF-7 cell line.



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A Study of Graph Invariants of Aramids

Umber Sheikh^{1*}, Ayesha Sattar¹

¹National Textile University, Faisalabad

**Email: umbersheikh@gmail.com*

Aramid admit significant applications in different fields. To quantify their physical characteristics be require the topological indices or graph invariants. This research is devoted to calculate some degree based topological indices (the first, second and modified Zagreb indices) of Aramids including Kevlar, Nomax and Technora. Moreover, the coefficients are found for the linear combination of graph invariants (the first, second and modified Zagreb indices) are estimated to predict the melting points of other aramids.

Keywords: Graph Invariants, Degree based Topological Indices, Aramids.



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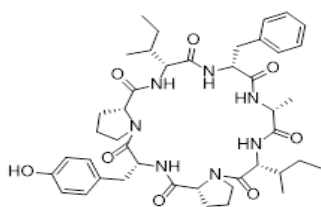
Solid-Phase Synthesis of Cyclic Peptide-Phakellistatin 18 and 21

Iqra Kanwal¹, Farzana Shaheen^{1*}

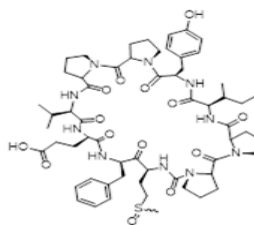
¹H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan

*E-mail: afnan.iccs@gmail.com

The cyclic peptides of phakellistatin family are proline rich and reported as potent anti-cancer compounds. So far, twenty-two members of phakellistatin were isolated from sponge of genus *Phakellia*. In current studies, two step solid-phase synthesis of phakellistatin 18 was performed, studies of linear precursor of phakellistatin 18 revealed it was produced as a mixture of inseparable conformer and new analogs were prepared by substituting all three proline residues by different amino acid residues. Cyclization of linear precursor of phakellistatin 18 and its new analogs was performed in solution phase. While phakellistatin 21 was obtained *via* on resin cyclization. All peptides were purified using RP-HPLC and their structures were confirmed by various spectroscopic techniques such as ESIMS, ¹H-NMR, ¹³C-NMR and HR-ESI-MS. *In vitro* anticancer screening of peptides was performed against different cancer cell lines. The linear precursor of phakellistatin 18 in which proline was substituted by lysine was found to be active against human breast cancer cell line. We aimed to further extend our studies to develop SAR studies of synthesized peptides.



Phakellistatin 18



Phakellistatin 21

Keywords: Phakellistatin, Cyclic Peptides, Proline-Rich Peptides, Solid-Phase Peptide Synthesis, Solution Phase Cyclization



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Synthesis of MBH Adduct Based Hydroxamic Acids Derivatives

Riffat Ullah^{1*}, Shafiullah Khan^{1*}, Hamid Ullah², Ghulam Mustafa²

¹*Institute of Chemical Sciences, Gomal University, D I Khan, KPK, Pakistan*

²*Department of Chemistry, Balochistan University of Information Technology, Engineering and Management Sciences, Quetta, Pakistan*

**E-mail: riffatullah.chemistry@gmail.com; shafi.ics.gu@gmail.com*

In the current research formation of five MBH adducts were prepared from aliphatic and aromatic aldehyde by treatment with ethyl acrylate, through a well-known MBH reaction. The pure MBH products were employed as synthetic precursors and thus converted into their respective four Hydroxamic acids with an exception that an aliphatic MBH adduct have not reacted. Chromatographic purification and then relevant spectral studies suggested their structural formulas. Thus a total of four Hydroxamic acids were prepared in good yield. The study inferred that aliphatic aldehyde based adduct resist to oximation however the aromatic aldehyde based adduct proved as good precursors for Hydroxamic acid formation. The study extended the synthetic potential of MBH adduct and broaden their scope as a precursors for derivatization. The study proposes that other aliphatic aldehyde based adducts can be investigated for their oximation into respective Hydroxamic acids to check whether all aliphatic aldehyde based adducts resist to oximation or not. The study also proposes formation additional derivatives of Hydroxamic acids can be prepared and biological investigation of the prepared Hydroxamic acids can exploit their biological potential.

Keywords: Synthesis, Characterization, MBH adducts, Hydroximation, Hydroxamic acids



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Efficient Liquid-Liquid Extraction of Phenolic Compounds from Model Oil using Benzyl Imidazolium Ionic liquids.

Nadiah Sidek^{1,2}, Ninie Suhana Abdul Manan^{1,2*}, Sharifah Mohamad^{1,2}

¹Department of Chemistry, University Malaya, 50603 Kuala Lumpur.

²University Malaya Centre for Ionic Liquid, University Malaya, Kuala Lumpur.

*Email: niniemanan@um.edu.my

Three benzyl imidazolium-based room temperature ionic liquids (RTILs) with various substituents namely allyl, benzyl, and vinyl were synthesized and used as solvents in liquid-liquid extraction for the removal of phenolic compounds from hexane as the model oil. The RTILs were characterized using ¹H NMR, ¹³C NMR, FT-IR, and CHN elemental analyses. Their density and viscosity were also measured. Five main parameters were evaluated through the removal process; the effect of IL substituent, the phase volume ratio of IL and model oil, phase contact time, and temperature. IL containing allylic substituent showed outstanding performance with approximately 95% efficiency under selected optimized conditions. To ensure that the RTIL can be used as a solvent for the removal of phenol, various other types of model oil apart from hexane such as petroleum ether, heptane, and cyclohexane were also used. The RTIL exhibited good recyclability and negligible loss of mass even after six cycles. Further mechanistic interactions between RTIL and phenol were studied by ¹H NMR and FT-IR.

Keywords: Room temperature ionic liquid, Benzyl imidazolium, Phenol, Liquid-liquid extraction, Model oil



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Improved Thermal Performance of Polyimides by Incorporation of Cardo and Trifluoromethyl Moieties.

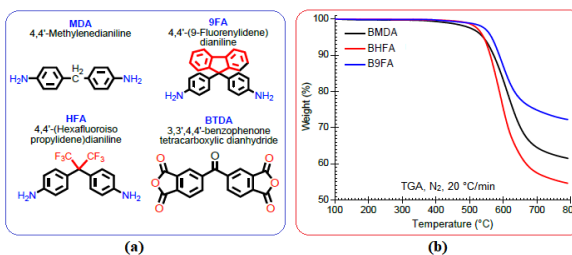
Ahmad Raza Ashraf^{1*}, Zareen Akhter², Muhammad Abid Rashid¹, Mian Habib Ur Rahman Mahmood¹

¹Department of Chemistry, University of Education, Lahore, Pakistan

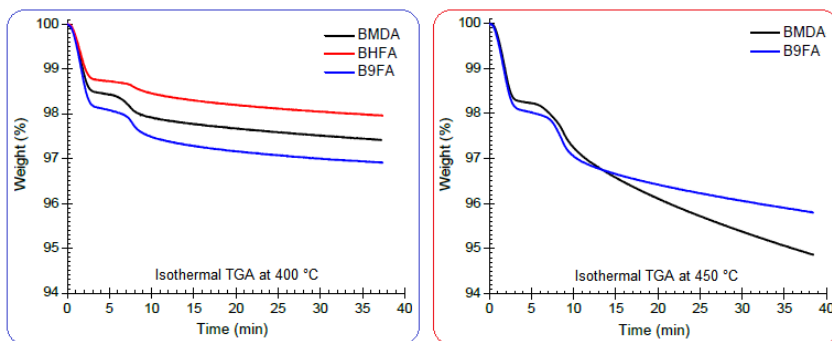
²Department of Chemistry, Quaid-i-Azam University, Islamabad, Pakistan

*Email: ahmad.raza@ue.edu.pk

Advances in the modern technologies are focused on reducing the cost of demanding industrial processes by replacing metals/ceramics with plastics. In this respect, polyimides are the materials of enormous scientific interest, attributed to several beneficial properties like outstanding thermal stability, excellent mechanical strength, chemical/radiation resistance, and low dielectric constant. Owing to these exceptional properties, polyimides have broad spectrum of applications in aerospace, automobile, electronics and various other industries as matrices, foams, coatings and gas separation membranes. Their properties are dependent upon the backbone structure, hence can be tailored/attuned to desired ones by modifying the structures of monomers used for their synthesis. The presented research reports the structure/property relationship of polyimides labelled as BMDA, BHFA, B9FA: derived from structurally related diamines and BTDA (Figure a). It involves the thermal measurements (dynamic/isothermal TGA, DMTA) to evaluate and compare distinct conditions relevant to application of polyimides with high thermal stability. It was observed that incorporation of cardo (B9FA) and trifluoromethyl (BHFA) moieties as pendant groups within the polyimide chain significantly improved the thermal stability/endurance (Figure b) and glass transition temperature of resulting polyimides. Hence, the developed polyimides have the potential for applications involving extended exposure at elevated temperatures ($\approx 400^\circ\text{C}$).



Keywords: Polyimides, Cardo, Trifluoromethyl, Thermal Performance



Isothermal TGA plots illustrating the effect of 9-fluorenylidene (B9FA) and trifluoromethyl (BHFA) moieties on thermal endurance of polyimides.

Highlights:

- Synthesis of polyimides for extended exposure at elevated temperatures.
- Improved thermal performance by cardo and trifluoromethyl moieties.
- Isothermal TGA for thermal endurance estimation.



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Synthesis and Characterization of Oximes Exhibiting Antibacterial Activity

Hamid Ullah^{1*}, Abdul Haleem¹, Riffat Ullah², Anjum Ayub³, Dilaraz Khan², Shafiullah Khan²

¹Department of Chemistry, Balochistan University of Information Technology, Engineering and Management Sciences, Quetta, Pakistan

²Institute of Chemical Sciences, Gomal University, D I Khan, KPK, Pakistan

³Department of Chemistry, NED University of Engineering and Technology, Karachi, Pakistan

*E-mail: hamidullah9@gmail.com; hamid.ullah@buitms.edu.pk

Oximes and related compounds are organic substances bearing “-C=N-OH” functionality. They are reported for their high structural diversities and strong biological activities. Chemically they can be transformed into almost all classes of organic compounds and inorganic complexes. The various chemical and biological significances justify Oximes as attractive structures for scientists. In the present research a series of aldoximes were prepared by treatment of the different aldehydes with $\text{NH}_2\text{OH}\cdot\text{HCl}$ under stirring and at room temperature upto 60°C . To obtain MBH adduct based ketoximes, initially MBH adducts were prepared as precursors which were then subjected to oximation. All the products were concentrated on rotary evaporator and then purified chromatographically. As a result a series of structurally diverse aldoximes and MBH adduct keto oximes were obtained in good to the excellent yield (70-92%) are shown in figure 1. All the Oximes were characterized through respective spectral analysis and performed antibacterial activity.

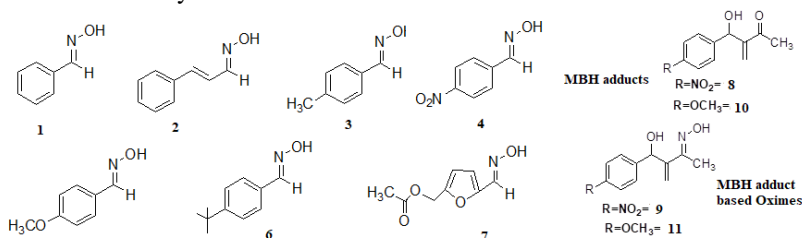
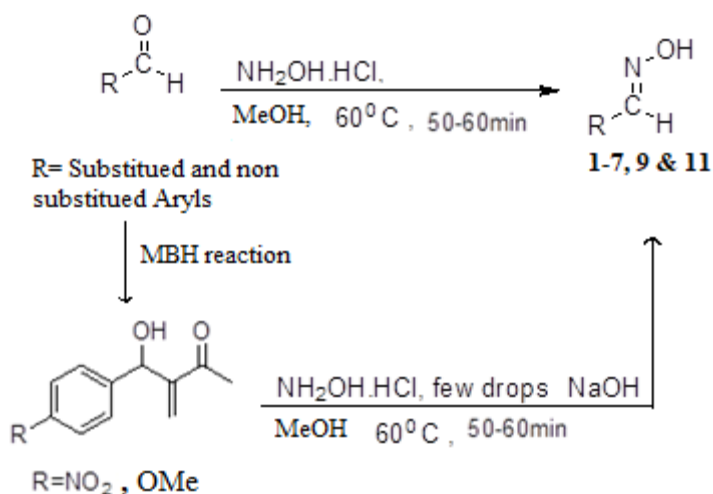


FIGURE 1. SYNTHESIZED OXIMES

Keywords: Aldehydes, MBH reaction, MBH adducts, Oximation, Oximes

Acknowledgement: ORIC BUIITEMS for financial grant number # 01/Research Projects/ORIC/BUIITEMS/2011/610.

References: [1] Ghozlojeh N. P., Setamdideh D. Orient. J. Chem., 31, 1823-1825 (2015). [2] Ullah H., Ferreira A.V., Bendassolli J. A., Rodrigo M. T., Formiga A., Coelho F., Synth. 47, 113-123(2013).



Highlights:

- Aldehydes were directly converted to Oximes
- Aldehydes were used to prepare MBH adducts as precursors which were subsequently converted into respective Oximes
- All the Oximes were investigated for their antibacterial activity



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Synthesis of the Antimicrobial Derivatives of Oleanolic Acid

**Nabila Hassan¹, Anjum Ayub^{1*}, Nuzhat Arshad¹,
Sabira Begum², Saima Tauseef³**

¹*Department of Chemistry, NED University of Engineering & Technology,
Karachi, Pakistan*

²*H.E.J Research Institute of Chemistry, International Centre for Chemical and
Biological Sciences, University of Karachi, Karachi, Pakistan*

³*Department of Microbiology, Federal Urdu University of Engineering &
Technology, Karachi, Pakistan*

**E-mail: anjumayub@neduet.edu.pk*

Natural products from medicinal plants provide unlimited opportunities for new drug leads. Due to an increasing demand for seeking therapeutic drugs from natural products, we synthesized some compounds. Herbal preparations for medicinal usage contain various types of bioactive compounds. The focus of our study is on the methodologies, which include the derivatization and characterization.

Oleanolic acid (3β -hydroxy-olean-12-en-28-oic acid), a penta-cyclic triterpenoid comprising a wide range of pharmacological and biological activities. It consisting three active sites the hydroxyl group C₃, double bond in between C₁₂ and C₁₃ and carboxylic group at C₂₈. Converting the C₂₈- carboxyl group to ester group led to different derivatives that showed nematocidal activity. Twelve derivatives of oleanolic acid have been prepared by converting the C₂₈- carboxyl group to ester group respectively. These were characterized by ¹H-NMR, UV and IR spectroscopy. Some of the compounds are reported for the first time. Parent compound along with derivatives were evaluated for their antimicrobial activity. Most of the compounds were found to be active against various Gram positive and Gram negative bacteria.

Keywords: Oleanolic Acid, Antimicrobial Activity, Gram Positive, Gram Negative



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Pharmacological Study of Bark & Leaves of *Syzygium Cumini* Used in Rustic Zones of Pakistan.

Uzma Shahid^{1*}, Syeda Rubina Gillani¹

¹Department of Chemistry, University of Engineering & Technology Lahore

*Email: 08.uetian@gmail.com

Syzygium cumini (jaman) is used as remedying at domestic level in rustic zones of Pakistan. An experiment to estimate the anti-microbial activity was conceded out at Department of Botany, University of Punjab Lahore. The phytochemical study was evaluated by using colored reactions on bark & leaves of *syzygium cumini* in Department of chemistry, University of Engineering & Technology Lahore. Antimicrobial activity was tested by using bacteria tagged as A, B, C, D. Fractions from *syzygium cumini* were applied on humans infected by diabetes, different problems of gum & teeth, skin. The bioactivity of bark & leaves of *syzygium cumini* is recorded on humans. Experiments have shown that bark & leaves of *syzygium cumini* have stronger role in soothing of diabetes, different problems of gum & teeth, skin. The extract of bark & leaves of *syzygium cumini* did not show any harmfulness on human health. The results confirmed that *syzygium cumini* has the antimicrobial activity & health benefits as medicinal plant.

Keywords: *Syzygium Cumini* (Jaman), Anti-Microbial Activity, Extract, Phytochemical Study.



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Simultaneous Determination of Citalopram with NSAIDs in Bulk Drug, Pharmaceutical Dosage Forms, and Human Serum by Validated RP-HPLC Method

Saeeda Nadir Ali¹, Nida Naz^{2*}, Amtul Qayoom¹,
Shumaila Akram³

¹Department of Chemistry, NED University of Engineering. & Technology,
Karachi, Pakistan

²Department of Applied Chemistry and Chemical Technology, University of
Karachi, Pakistan

³Department of Chemistry, University of Karachi, Pakistan
*E-mail: na.msichem@gmail.com

A high-performance liquid chromatography method was designed and validated to quantify citalopram simultaneously with piroxicam, celecoxib, and diclofenac sodium. Chromatographic evaluation was performed at ambient temperature utilizing Shimadzu Shim-Pack CLC-ODS (M) 25M column connected to UV-visible detector operated at 230 nm using methanol: Water (pH 3.5) as the mobile phase having composition 80:20 (v/v) flowing at rate of 1.0 mL min⁻¹. The validation was carried out in the ranges 0.6-20, 0.9-28, 0.6-20 and 1.0-32 µg mL⁻¹ with lowest value corresponding to detection limit 16.45, 23.33, 27.66 and 14.44 ng mL⁻¹. Inter day precision ranged from 0.14-1.67% and intraday precision from 0.40-1.50% with accuracy ranged 99.61-100.86%. The reported drugs were effectively detected deprived of interference in commercial formulation and human serum, exhibiting efficacy of developed method.

Keywords: Citalopram, NSAIDs, Validation, Method Development, RP-HPLC.



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IICC21-P-45



Study of Physico-Chemical Parameters of Varieties of Joshanda Decoction with Respect to Consumer's Health

Rubina Parween¹, Bushra Shamshad^{1*}, Zainab Jehan¹

¹*Department of Chemistry, Faculty of Sciences, Federal Urdu University of Arts, Science and Technology, Karachi, 75300, Pakistan*

**E-mail: bushra.shamshad@fuuast.edu.pk*

Joshanda is extensively used in Pakistan as a remedy for relief in cough and flu. This research work was conducted in dual segments on samples of commercially available instant Joshanda of various brands having different flavors. Initially, samples of herbal decoction were prepared and their physicochemical properties (pH, TDS, conductivity, and specific gravity) were recorded. Subsequently, study explored for the determination of the total content of mineral oxides and levels of some essential metals such as sodium (Na), potassium (K), calcium (Ca) and Iron (Fe). This task was accomplished by wet digestion of samples decoction. The concentration of electrolytes (Na and K) and trace metal (Fe) were assessed by flame emission spectroscopy (FES) and atomic absorption spectroscopy (AAS) respectively. While strength of Ca was measured through complexometric titration. The results were statistically analyzed and compared with RDA guidelines established by National Research Council (USA) and accessible literature. Moreover, the obtained results of physicochemical parameters (pH, conductivity, TDS, specific gravity) revealed that the locally available instant Joshanda is good for health since it is mildly acidic and a safe remedy in flu and cough for ulcer patients as well.

Keywords: pH, Conductivity, Electrolytes, Calcium, Iron



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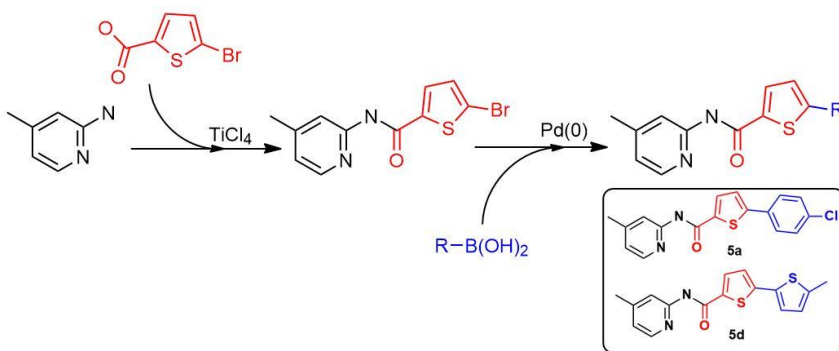
Synthesis of Pyridine based Carboxamide Derivatives and their *In-Vivo* Anticonvulsant Activity

**Muhammad Bilal^{1*}, Nasir Rasool^{1*}, Gulraiz Ahmad¹,
Iram Kanwal¹, Musrat Shaheen¹**

¹Department of Chemistry, Government College University Faisalabad,
Faisalabad 38000, Pakistan.

*Email: nasirrasool@gcuf.edu.pk, muhammadbilalgcuf@gmail.com

Aminopyridine derivatives exhibit several biological activities and take a key position in the pharmaceuticals. In the present study, the 5-Bromo-N-(4-methylpyridine-2-yl)thiophene-2-carboxamide was synthesized by direct amidation of thiophene carboxylic acid and aminopyridine via TiCl_4 in a good yield (80%). Then the arylation of synthesized carboxamide was done by $\text{Pd}(0)$ Catalyzed Suzuki-Miyaura Cross-Coupling reaction under inert environment. It gave fair to good yields (35-84%) of the synthesized derivatives. The anticonvulsant activity of the synthesized compounds was observed in-vivo. The compound **5a** and **5d** exhibited a potential anticonvulsant activity.



Keywords: Aminopyridine, Carboxamide, Suzuki-Miyaura, Cross Coupling, Arylation, Anticonvulsant



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Urease Inhibition Activity of Transition Metal Chelates: Anti-ulcer Agents

Noshab Qamar¹, Hira Sultan², Ahmed³, Maria Ashfaq¹, Raheela Naz¹, Rafia Azmat¹, Mehreen Lateef⁴, Khalid Mohammed Khan^{5,6}, Tanzila Arshad⁷

¹ Department of Chemistry, University of Karachi, Karachi, Pakistan

² Department of Chemistry, NED University of Engineering and Technology, Karachi, Pakistan

³ Quaid-e-Azam University, Islamabad

⁴ MDRL, Baharia University of Medical & Dental College, Karachi, Pakistan

⁵ H. E. J. Research Institute of Chemistry, International Center of Chemical and Biological Sciences (ICCBS), University of Karachi, Karachi, Pakistan

⁶ Department of Clinical Pharmacy, Imam Abdulrahman Bin Faisal University, Dammam, Saudi Arabia

⁷ Department of Applied Chemistry and Chemical Technology, University of Karachi, Pakistan

*E-mail: noshabqamar@gmail.com

In the current work, in-vitro urease inhibition activity of metal heterochelates of Cr (III), Mn (II), Fe (III), Co (II), Ni (II), Cu (II), Zn (II), Cd (II) and Pb (II) with 8-hydroxyquinoline and *DL*-methionine has been presented with their docking study. These complexes were already reported for their excellent anti-oxidant activity. All the complexes showed urease inhibition activity, while thiourea was the standard having IC₅₀ value $21.6 \pm 0.12 \mu\text{M}$. Among the nine complexes, it was found that Cu (II) complex showed potent inhibitory activity ($22.6 \pm 0.72 \mu\text{M}$) comparable with the standard thiourea ($21.6 \pm 0.12 \mu\text{M}$). Mn (II), Fe (III), Cd (II) and Pb (II) also showed better inhibitory. A docking analysis was used to explain the inhibitory activities of complexes.

Keywords: Urease, inhibition activity, complexes, docking.



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Spectrophotometric Determination of Antihistamines by Charge Transfer Complexes

**Saman Naeem^{1*}, Saeeda Nadir Ali², Amtul Qayoom²,
Haji Muhammad³, Shazia Nisar⁴**

¹*Bahria College, EAB-1 Majeed SRE, Karachi*

²*Department of Chemistry, NED University of Engineering and Technology, Karachi.*

³*Department of Chemistry, Federal Urdu University of Arts, Sciences and Technology, Karachi.*

⁴*Department of Chemistry, University of Karachi, Pakistan.*

**Email: ms_saman@outlook.com*

The current investigation was carried out to develop a simple and rapid spectrophotometric method for the determination of selective antihistaminic drugs via charge transfer complex with curcumin. The method validation has been accomplished by observing the optimum conditions for the reactions that obeyed Beer's law with correlation coefficient greater than 0.9981 in each case. The effective implement of proposed method was attained for the determination of antihistaminic drugs in pharmaceutical formulations. The reliability of method without interference of excipients was conferred by satisfactory recovery values. Additionally, the spectral characteristics including oscillator's strength, dipole moment, ionization potential, energy of complexes, resonance energy and also the thermodynamic parameters i.e. association constant and Gibb's free energy changes have been determined. Benesi-Hildebrand plots for each complex have been constructed. In addition, solid charge transfer complexes of all five antihistamines were synthesized and characterized by IR spectroscopy.

Keywords: Charge Transfer Complexes, Antihistamine, Benesi–Hildebrand Plot



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ICC21-P-49



***In-Vitro* Interaction Studies of Antiviral Drugs with Nsaids by Liquid Chromatography: Application in Pharmaceutical Formulation and Human Serum**

**Syed Muhammad Bilal Ali¹, Saeeda Nadir Ali¹,
Muhammad Raza Shah², Muhammad Saad**

¹*Department of Chemistry, NED University of Engineering. & Technology, Karachi, Pakistan*

²*International Center for Chemical and Biological Sciences, University of Karachi, Pakistan*

³*Department of Chemistry, University of Karachi, Pakistan*
**E-mail: saeeda@neduet.edu.pk*

A simple, rapid and precise HPLC method was developed for the simultaneous method of Ledipasvir, Sofosbuvir and Diclofenac. The method is also validated according to ICH guidelines consisting Linearity, Accuracy, Precision and Robustness. The method was optimized on 0.1% Phosphoric Acid:Methanol at 45°C column temperature at 1ml/min flow rate with gradient mobile phase Using C₁₈ Column having length 150 x 3.9mm and pore size of 5µm. All the three drugs were analyzed by UV detector at 249nm wavelength. All three Drugs were separated within 12 min of Run time. Furthermore, the method is also applied on Pharmaceutical Formulation and as well on Serum Samples. And the results obtained by them were found to be linear. Interaction Study was also conducted on three mediums 0.1N HCl, Buffer pH 4.5, and Buffer pH 6.8 at all three mediums Drug was dissolved 85%. The Method is also optimized by Design of Experiments on Central Composite Design which also suggest that the method is suitable for all three drugs. Hence, the method is all suitable for Bioequivalence as well as in Pharmaceutical Manufacturing.

Keywords: HPLC, Simultaneous, Ledipasvir, Sofoubuvir, Diclofenac.



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Development of a Unique Homeopathic Cosmetic Formulation for Hair Growth and a Powerful Neuroprotective Gland Stimulator

Sofia Naureen¹, Simra Ashfaq¹, Nudrat Nawab¹, Maneha Imran¹, Wajeeha Waseem¹, Muhammad Ali Versiani¹, Sajid Jahangir¹, Kehkashan Khan^{1*}

¹Department of Chemistry, Federal Urdu University of Arts, Science and Technology, Karachi, 75300, Pakistan

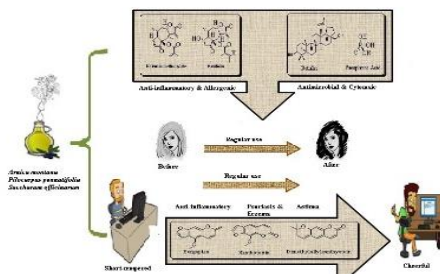
*E-mail: kehkashan.khan@fuuast.edu.pk

Malnutrition and stress may lead to rough skin and loss of mental health. Similarly, polluted environment is one of the major root causes of nasal polyps which eventually results in hair fall, greyish or white hairs and insomnia for a large number of people. Hence, present study unveils antioxidant potential of *Arnica Montana* (whole plant), *Pilocarpus pennatifolius* (flower) and *Saccharum officinarum* (Sugar cane vinegar) liquor for hair treatment and neuroprotective effects. To the best of our knowledge, this is a first formulation developed with dual mode of action for the treatment of hair and mental stress. The uniqueness of this formulation lies in its dual target of cosmetic and medicinal effects. Our developed formulation exhibits healing, anti-inflammatory, and neuroprotective potential against scalp disorders. Moreover, its dual effect may be due to the presence of antioxidant phytochemicals including phenolics, flavonoids, etc., in these plants.

Keywords: Neuroprotective, Hair fall, Cosmetics, Phenolics, Flavonoids.



- Herbal extracts
- Neuroprotective effect
- Cosmetic effect





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Under Investigation Symptom-Based Development of Herbal Formulation for the Treatment of Covid-19

Maha noor¹, Hakeem Noor Muhammad², Syed Haider Jaffri¹, Muhammad Usman Younus¹, Ghazanafar Abbas¹, Jahanzaib Liaqat Ali¹, Nadia Naz¹, Muhammad Ali Versiani¹, Sajid Jahangir¹, Kehkashan Khan^{1*}

¹Department of Chemistry, Federal Urdu University of Arts, Science & Technology, Karachi, Pakistan

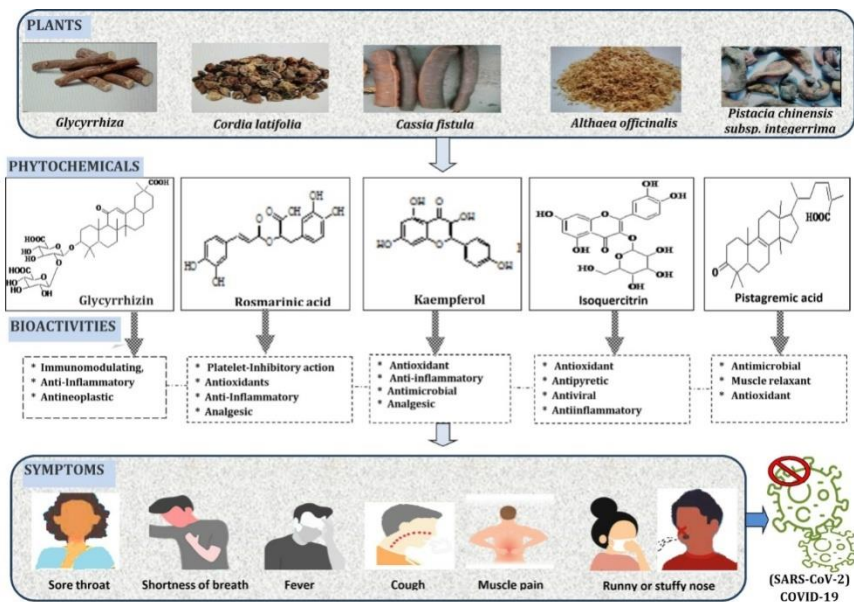
²Hamdard University, Karachi, Pakistan

*E-mail: kehkashan.khan@fuuast.edu.pk

Recently evolving global pandemic of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) with no clinically accepted medication yet prompted us to investigate traditional medicinal plants for its cure. It is the modified Ayurveda formulation which has been applied on thousands of patients for the treatment of pandemic Influenza virus several decades ago in India. Moreover, the common symptoms shared between Influenza and Coronavirus, provided baseline for this formulation. Pneumonia, fever, dry cough, tiredness, sore throat and chest pain are some of the most common symptoms observed in COVID-19 patients. Hence, therapeutic effects of five miracle plants including *Pistacia chinensis subsp. integerrima* (J. L. Stewart ex Brandis), *Althaea officinalis*, *Cassia fistula*, *Cordia latifolia* and *Glycyrrhiza glabra* applied during Influenza virus pandemic with immunomodulatory and immune-stimulatory effects have also been identified as potential candidates against COVID-19 symptoms. Herbal medicines consist of several phytochemicals rather than single compound and exhibit less side effects. Aforementioned miracle plants exhibit antiviral, immunomodulatory, immune-stimulatory, analgesic, anti-microbial, antioxidant, and anti-inflammatory effects due to the presence of several phytochemicals including polysaccharides, flavonoids, tannins, triterpenes etc. Hence, this under investigation formulation can be an effective herbal remedy for Covid-19 patients.

Keywords: COVID-19, Anti-viral, Herbal formulation, Immunomodulatory, Antioxidant

Graphical Abstract:



Highlights:

- Under Investigation Symptom-based Development of Herbal Formulation
- Common Symptoms of Influenza and Covid-19
- Antiviral



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IICC21-P-52



Investigation Process of Pharmaceutical Drug Recall

Muhammad Younas¹, Abid Ali¹, Anum Irfan¹, Mubashir Hussain¹, Muhammad Ali Versani^{1*}, Muhammad Sajid Jahangir^{1*}, Kehkashan Khan^{1*}

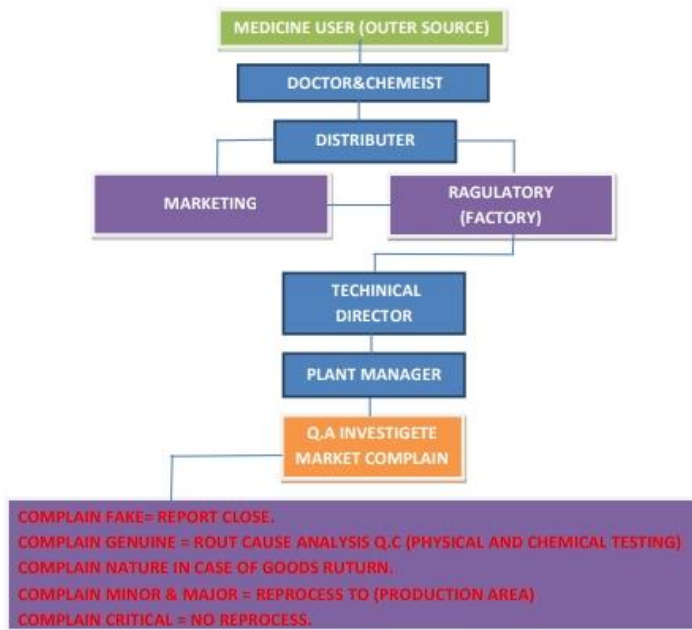
¹Department of Chemistry, Federal Urdu University of Arts, Science & Technology, Karachi, 75270, Pakistan

**E-mail: mali.versani@fuuast.edu.pk, sajid.jahangir@fuuast.edu.pk, kehkashan.khan@fuuast.edu.pk*

Healthcare system is one of the basic issues, both for the developed and the developing countries too. In this regard, Pharmaceutical Drug Recall (PDR) plays a crucial role in monitoring and maintaining public health. PDR is the collection of marketed sub-standard, wrongly analyzed/stored, mishandled drugs, etc., back to the company it manufactures. Market complaints and drug side effects are equally responsible for it. Failure of PDR may give birth to moral, social, religious, mental, financial and hygiene issues. European countries deal it very effectively and punish the responsible company through different penalties including huge amount of fine, etc. Similarly, “Medicine Board” of different countries monitors this issue through patient and market survey, and deals as per law. On the contrary, this is not the case in developing countries. This may be because of the relaxed law practicing conditions, poverty, poor economic status, etc. FDA and DRAP shares drug recalls in USA and Pakistan, respectively. Moreover, recollection of sub-standard drug from the market may be a temporary financial loss for the company but it gets good market reputation in return. Conclusively, strict implementation of law at governmental level may control this issue in developing countries too.

Keywords: Drug recall, Regulatory bodies, Recall strategy, Quality, Safety.

ORGANIZATIONAL CHART



Highlights:

There are two types Recollection.

- Voluntary Recall
- Statutory Recall

Synthesis of Chiral Thiadiazine Thione with their Antiulcer and Antioxidant Activity.

**Shumaila Jawaid¹, Nuzhat Arshad^{1*}, Anjum Ayub¹,
Jamshed Hashim², Mehreen³**

¹Department of Chemistry, NED University of Engineering. & Technology,
Karachi, Pakistan

²H.E.J. Research Institute of Chemistry, International Center for Chemical and
Biological Sciences, University of Karachi, Pakistan

³Multidisciplinary Research Lab, Bahria University Medical and Dental
College, Bahria University, Pakistan

*E-mail: nuzhat@neduet.edu.pk

Five novel chiral Thiadiazine Thione were directly synthesized by using chiral amines i.e. S-(-)-alpha-methyl benzyl amine and R-(+)-1-phenylethyl amine with single pot synthesis. The obtained products were identified through NMR Spectroscopy, Mass Spectrometry and evaluated for their in vitro urease inhibitory activity and antioxidant activity. These chiral compounds were first time examined for urease inhibition and anti-oxidant activity. These chiral compounds were found to be significantly active with IC₅₀ values between 30.5-34.8 μ M, in comparison of thiourea against antiulcer activity while moderately active within the range of IC₅₀ values 57.8-69.9 μ M when compared with the standard BHA (IC₅₀=44.2 μ M) against antioxidant activity.

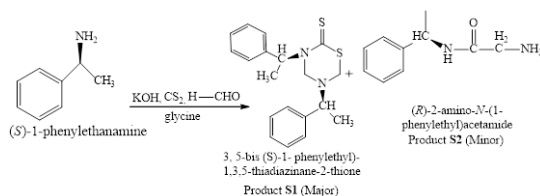


FIGURE 1: SYNTHESIS OF CHIRAL THIADIAZINE THIONE

Keywords: Chiral, Thiadiazine Thione, Urease inhibitory activity, Antioxidant.



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Synthesis and *In-Vitro* Antimicrobial Screening of Benzimidazole Conjugated Peptides

**Husena Aamra¹, Munira Zafar², Humera Jahan², Hunain Ali¹,
Serab Khan¹, Farzana Shaheen^{1*}**

¹*H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan*

²*Dr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan*

**E-mail: afnan.iccs@gmail.com*

In recent years, the incidence of microbial infections has increased significantly. Currently available antibiotics have lost their efficacy and specificity towards several bacterial strains due to the development of resistance against them. Gastroenteritis is one of those bacterial infections which is associated with multidrug resistance gram-negative bacteria *Salmonella typhimurium*, which has high prevalence and mortality rate, especially in developing countries. Antimicrobial peptides are the vital constituent of innate immune system and are reported to have high specificity. Cationic antimicrobial peptides serve as an eminent template for the designing and development of peptide based therapeutics. In this study we describe a study on the synthesis and bioactivity of small library of novel short cationic antimicrobial peptide-benzimidazole conjugates. The peptide-benzimidazole conjugates were prepared on Wang resin from C to N terminus followed by capping with benzimidazole using SPPS by Fmoc strategy. The detailed structural studies of all peptides were performed by using ESI-MS, ¹H- NMR, ¹³C-NMR, and HR-FABMS. The antimicrobial potential of these peptide-benzimidazole conjugates were investigated against a multidrug resistant clinical isolate *Salmonella typhimurium*. Our results showed that the two new conjugates with cationic groups were identified as inhibitors of *Salmonella typhimurium* UMR1 strain.

Keywords: Gastroenteritis; *Salmonella typhimurium*; peptide-benzimidazole conjugates; multidrug resistance; Cationic antimicrobial peptides.



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IICC21-P-55



Effective Treatment of Dye Contaminated Aqueous Solution from Bark of *Guaiacum officinale* “A Low Cost Effective Adsorbent”

Ghazala Aftab¹, Hira Sultan¹, Ghazanfar Hussain²

^{1, 2}NED University of Engineering and Technology

*Email: ghazala_aftab@live.com

Synthetic dyes are present in waste water effluent, it is considered as a source for an impending hazard to the environment hereafter it is essential to remove such dyes from water bodies. Chemical, Physical, and Biological methods are used as a removal technique for these dyes. In all these removal techniques adsorption is considered as one of the most cheapest and effective method. Consequently, studies allied to probing for efficient and low cost adsorbents resulting from existing resources are seeking attraction for removal of dyes. Experimental studies showed that there are various non-conventional low cost adsorbent have been used for the removal method. Bark of the tree (*guaiacum officinale*) was found to be effective for the removal of methylene blue and malachite green from the water. The suitable pH is 7 for the removal of 50 ppm of methylene blue and malachite green from aqueous solution. 0.2 g of adsorbent dosage was selected for maximum removal of both the dyes in 30min. 89% removal was achieved for MB and MG at these optimal conditions.

Keywords: Dyes, Adsorption, Low cost adsorbents.



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Phase Behavior Measurement and Flash Calculations for Hydrate Formation and Dissociation Temperature for Ethane + Propane + Water System

**Khan Muhammad Qureshi^{1*}, Saima Khan², Sami Chana³,
Zulfiqar Ali Solangi¹**

¹*Chemical Engineering Department Mehran University of Engineering and Technology Jamshoro, Pakistan.*

²*Department of Chemical Engineering, University of Malay, Kuala Lumpur Malaysia.*

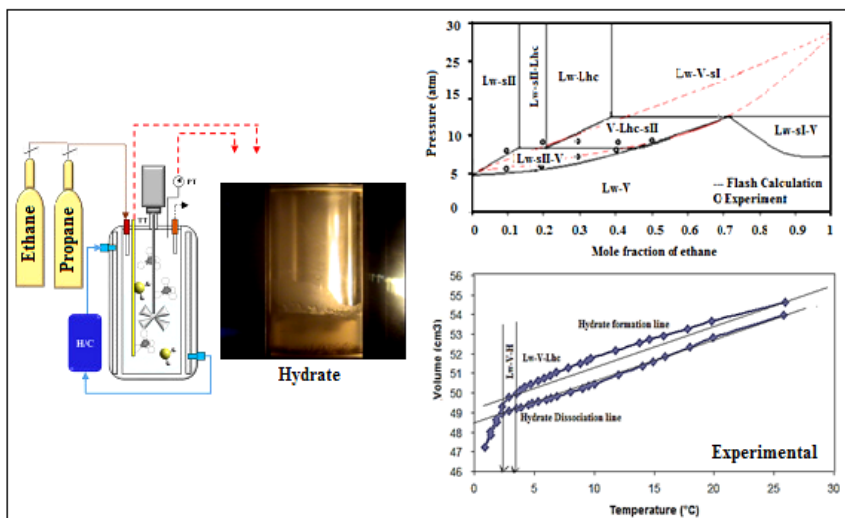
³*Quaid-e-Awam University of Engineering, Science and Technology, Nawabshah, Pakistan.*

**E-mail: khan.muhammad@faculty.muet.edu.pk*

This study is aimed to investigate the occurrence of pseudo retrograde hydrate behaviour in ternary systems. Flash calculation and equilibrium points were measured of ternary system ethane, propane and water system were determined at 277.9K, 278K and 280K. Structure sI and sII hydrates were formed at various concentrations of ethane, propane and water system ranging from 0.1-0.9 mole fractions. Flash calculation presented that the increase in temperature or mole fractions of ethane decreased the hydrate formation rate. It is also observed that increase in mole fractions of propane served as an inhibitor in the formation of sI hydrate. Furthermore, no evidence of pseudo retrograde hydrate behaviour is not predicted experimentally and with flash calculations in ternary system.

Keywords: Phase behaviour, Flash calculation, Pseudo retrograde, Dissociation.

Graphical Abstract:



Highlights:

- To investigate the occurrence of pseudo retrograde hydrate behaviour in ternary systems.
- Flash calculation and equilibrium points were measured.
- No evidence of pseudo retrograde hydrate behaviour is not predicted.



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Micellar Enhanced Ultrafiltration (MEUF) for Removal of Rhodamine B (RhB) from Aqueous System

Muhammad Usman^{1*}, Amnah Yusaf¹

¹*Department of Chemistry, GC University, Faisalabad, Pakistan*

**Email: usm_ca@yahoo.com*

Micellar enhanced ultrafiltration (MEUF) has proved itself to be a potentially attractive tool to remove contaminants from waste water. The reported study is particularly focused on the interaction and removal of cationic dye, Rhodamine B (RhB), using micellar solution of anionic surfactants i.e. Sodium dodecyl sulfate (SDS) and Sodium Oleate (SO). Dye removal efficiency has been assessed in terms of rejection percentage and permeate flux, using cellulose membrane of 10,000 molecular weight cut off (MWCO). The effects of various factors i.e. ionic strength, concentration of dye, concentration of surfactants, concentration of electrolyte, pH, operating pressure and rotations per minute (RPM) has been observed. It has been concluded that the maximum rejection of dye has been observed using micellar media of SDS. Overall, it has been observed that the rejection coefficient of dye is higher at higher concentration of surfactants and electrolyte and at lower values of pH, RPM and transmembrane pressure.

Keywords: Micellar Enhanced Ultrafiltration, Rhodamine B



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Study of Different Interactions of Thiamine Hydrochloride in Aqueous, Aqueous Methanol and Aqueous Ethylene Glycol Systems by using Masson's and Jones-Dole Equation

Zainab Khan¹, Summyia Masood^{1*}

¹Department of Chemistry, University of Karachi, Pakistan

*E-mail: smasood@uok.edu.pk

This work reports volumetric and viscometric properties of drug thiamine hydrochloride in aqueous and aqueous alcoholic systems (aqueous methanol and aqueous ethylene glycol) at different temperatures (298.15-318.15) K. Densities of drug solutions were used to calculate apparent molar volume (ϕ_v) for different concentrations (0.04-0.14 mol.dm⁻³) of drug in aqueous, aqueous methanol and aqueous ethylene glycol (10% v/v) systems at different temperatures. The limiting apparent molar volumes (ϕ_v^0) and experimental slopes (S_v) derived from the Masson equation, and explained in terms of drug-solvent and drug-drug interactions, respectively. The partial molar expansibilities were also evaluated which indicate presence and absence of caging or packing effect. The structure breaking and structure making properties of drugs has been discussed with the help of Hepler's criterion ($\partial C_p / \partial P$)_T. Moreover constants of Jones-Dole equation were calculated from viscosity measurement which supported the results obtained from volumetric study.

Keywords: Density, Viscosity, Apparent Molar Volume, Drug-Solvent Interactions, Thiamine Hydrochloride.



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Dispersive Solid Phase Extraction of Traces Lead on CuCo_2O_4 Adsorbent from Environmental and Food Samples

Furkan Uzcan^{1,2}, Mustafa Soylak^{1,2}

¹Department of Chemistry, Erciyes University, Kayseri, Turkey

²Technology Research and Application Center, Erciyes University,
Kayseri, Turkey

*E-mail: furkanuzcan@erciyes.edu.tr

CuCo_2O_4 nanoparticle has been firstly used as solid phase extractant for the dispersive solid phase extraction of lead (II) in the presented work. Analytical parameters, such as pH, eluent type and volume, adsorbent amount, adsorption-desorption contact times, sample volume, which are effective on the recovery of the method have been optimized. While the preconcentration factor was calculated as 25 times, the detection limit (LOD) was found as 6.55 $\mu\text{g/L}$. The accuracy of the method was checked by applying the method to TMDA 53.3 water certified reference material. The presented dispersive solid phase extraction method was successfully applied to various food and environmental samples.

Keywords: Dispersive Solid Phase Extraction; CuCo_2O_4 Nanoparticles; FAAS; Food



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IICC21-P-60



Separation-Enrichment of Trace Levels of Cu (II) Ions by Dispersive Solid Phase Microextraction on Modified Ni-Fe@ACC

Seda Duman^{1*}, Mustafa Soylak¹⁻²

¹ *Department of Chemistry, Erciyes University, Kayseri, Turkey*

² *Technology Research and Application Center, Erciyes University, Kayseri, Turkey*

**E-mail: duman58seda@gmail.com*

While copper, one of the heavy metals, is of vital importance due to its duties in the biological systems of living things, on the other hand, high doses cause serious problems due to its toxicity. So, it is of great importance that copper, which is released into the environment and accumulates on biological/environmental samples, is determined by accurate, environmentally friendly and fast analytical methods due to its fundamental importance and dangerous effects on the ecosystem and living things. In this study, a SPME method has been developed in which using modified activated carbon fabric as adsorbent for separation-preconcentration of Cu (II) ions. Cu (II) ions were detected using microinjection with FAAS. With the reaction carried out in the hydrothermal synthesis unit, the activated carbon fabric was coated with Fe and Ni metals and bimetallic nano structures were obtained, characterized by using SEM and FTIR. Important analytical parameters such as pH, adsorbent amount, eluent concentration and volume, sample volume, matrix effect were optimized. At pH 9.0, the enrichment factor of the method developed using 5 mg of adsorbent was calculated as 40. The validation of the method was verified by addition recovery test of Cu (II) ions on various real samples.

Keywords: Copper; Solid Phase Microextraction; Ni-Fe@ACC; FAAS



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Study of Exports and Imports in Textile Hosepiping, Similar Textile Tubing, with or without Lining, Armor or Accessories of other Materials of Pakistan

Muhammad Ali¹, Ibrahim¹ and Danish Hassan^{2*}

¹*Department of Textile & Clothing, National Textile University, Karachi*

²*Department of Applied Sciences, National Textile University, Karachi*

**Email: ali.ikhtiar406@gmail.com, Ibrahim.khan9718@gmail.com,
danish10ansari@gmail.com*

Pakistan is an agriculture country and a great producer of cotton among the different countries. The exports and imports (2010-2019) of Pakistan in textile tubing, hosepiping and other such textile materials were discussed in that paper in value (US\$) by use of statistical tools like central tendency and coefficient of variation so, the results show the imports of Pakistan in textile hosepiping, armor or other materials for past ten years is greater than exports and the imports are normal distributed year by year as compared to exports. The normal tendency and least coefficient of variation of imports depicts the long term continuation.

Keywords: Textile HosePiping, Tubing, Lining, Armour, Coefficient Of Variation.



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Mechanistic Modeling of Cyclic Voltammetry and EIS: A Useful Tool for Understanding Biosensor Principles.

**Syed Muhammad Ali Rizvi¹, Shazia Perveen^{1*}, Muzamil Jalil¹,
Wahaj Ejaz¹, Arsalan Ahmed Khan¹**

*¹Department of Chemistry, NED University of Engineering and Technology,
Karachi.*

**Email: shaziaperveen@neduet.edu.pk*

Electrochemical sensors have attracted considerable attention for the sensitive detection of a variety of biological and pharmaceutical compounds. Carbon-based nano-materials including carbon nanotubes, C₆₀ and graphene have gained tremendous interest in the design of high-performance electrochemical sensor platforms. Electrochemical biosensor have exceptional thermal, mechanical, electronic, and catalytic properties. Electrochemical detection of analyte is a very elegant method in analytical chemistry. Electroanalytical methods have lot of advantages such as simplicity, low cost, short time of operation, high sensitivity, and availability of in-situ monitoring. Main features of these techniques are sensitivity, specificity and cost-effective detection. These parameters are critical for the high-quality sensing technology. The modern era requires combination of technological and biological approaches for more and more satisfactory devices. Electrochemical biosensors have found application in many fields, they offer rapid and very sensitive analysis in real-time. Electrochemical techniques, mainly voltammetric and Electrochemical Impedance Spectroscopy (EIS), are novel techniques due to their wide range of target analyte detection.

Keywords: Mechanistic modeling, Cyclic voltammograms, Electrochemical Impedance Spectroscopy, Amperometric biosensors



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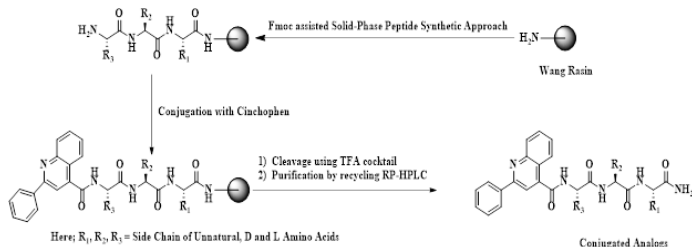
Synthesis and Biological Studies of Cinchophen-Conjugated Peptides

Anila Bashir¹, Arif Iftikhar Khan¹, Farzana Shaheen^{1*}

¹H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan

*E-mail: afnan.iccs@gmail.com

Millions of people yearly died by different cancers. Treatments available for cancer are invasive or very costly yet doesn't guarantee life. Chemotherapeutics available for treatment of cancers are non-specific affect normal cells leading to various side effects. Peptides have great pharmacological importance being selective in nature and having safe mode of action. But peptide therapeutics have some limitations such as proteolytic degradation in acidic environment. It is reported that conjugation of some active heterocycles and some unusual amino acid residues may increase the stability of peptides. Cinchophen (2 phenylquinoline-4-carboxylic acid) an active therapeutic molecule and its peptide conjugates are reported to enhance biological potential. Currently, we designed cinchophen conjugated peptidomimetics having unusual amino acid residues. These peptide conjugates synthesized using Fmoc-assisted SPPS methodology. Synthetic peptides were characterized by different spectroscopies and their biological evaluation against different cell lines is under process to find some lead molecules.



General Synthetic Scheme of Solid-Phase Synthesis of Cinchophen Conjugated Peptides

Keywords: Pharmacological importance; Unusual amino acid; Solid phase peptide synthetic (SPPS); proteolytic degradation; Peptidomimetics.



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Electrochemical Water Treatment for Drinking Purposes

Ufaq Zehra^{1*}, Zahoor Ahmed^{2*}

¹Department of Chemistry, University of Engineering and Technology Lahore,

²Department of Chemical Engineering and Technology, University of Engineering and Technology Lahore, Pakistan

*Email: ufaqzehra5@gmail.com, zahoorchem@uet.edu.pk

Inadequate availability of healthy and safe drinking water is a critical challenge faced by millions of people in third world countries. Herein, a new blend of conventional water treatment process has been proposed in which water can be treated electrochemically in a 10 liter batch reactor of aluminum, steel and copper electrodes.

After treating the water through electrochemical reactor, various parameters like pH, conductivity, turbidity, total dissolved solids, total suspended solids, hardness test, chloride tests, sulphate test and total bacterial count were observed and compared with WHO standards to determine the quality of treated water. Obtained results revealed that the maximum energy consumption for using the aluminum and copper electrodes is 4.91 and 4.31 KWh/m³, respectively at current density of 1.25 mA/cm² and 30 minutes operating time. This study did not involve toxic chemicals and large amount of electricity. So, it would be new addition in current state of knowledge and considered as cost effective and facile process for water disinfection as shown below:

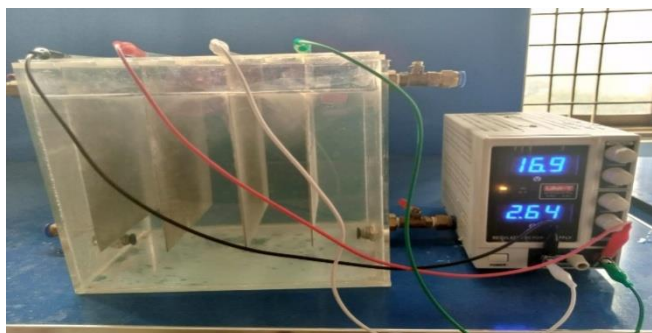


FIG. 1