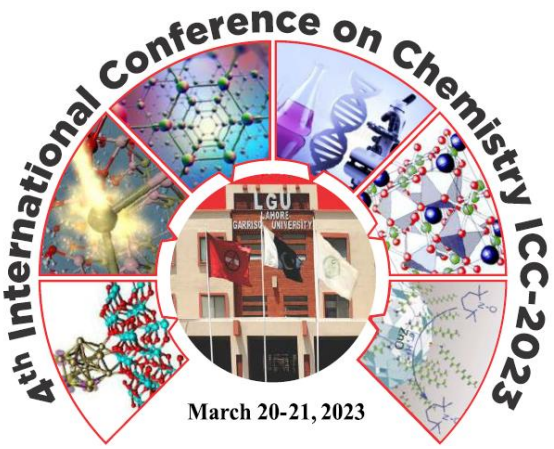
# Proceedings of
# 4th International Conference on Chemistry ICC-2023 Hybrid Mode

## Theme:
## Modern Trends in Chemical, Biological and Material Sciences

**March 20-21, 2023**

# ABSTRACT BOOK




**Organized By: Department of Chemistry, LGU Lahore**

http://icc.lgu.edu.pk

# Modern Trends in Chemical, Biological and Material Sciences

**March 20-21, 2023**

## Venue: Jinnah Auditorium, Iqbal Auditorium and Usman Shoukat Hall

**Organized By: Department of Chemistry, Lahore Garrison University Lahore**

## WELCOME TO ICC-2023

Lahore Garrison University (LGU), Department of Chemistry announces the 4th International Conference on Chemistry (ICC-2023) Hybrid Mode, Entitled: Modern Trends in Chemical, Biological and Material sciences to be held on March 20-21, 2023. This two day conference 4th in the series will bring together researchers from industry, academia and government and non-government organizations to discuss the state-of-the-art, and recent advancements in the field of chemical, biological and material sciences. The conference will be Gordon Conference style, with discussion sessions and panels, to allow extensive interactions among participants. We cordially invite all the participants who are interested in sharing their knowledge. The conference will address and harmonize the advancements in science and technology to achieve the sustainable development goals for uplift of education and research in developing countries.

Initially, at the first place we are thankful to Lahore Garrison University, which have supported the organizing of the conference at all levels. Without the great devotion of our faculty and administrative staff of the university, it would simply have been impossible to organize this esteemed event.

We are very grateful to all participants from different cities and countries attend the conference. We wish you all a very pleasant and inspiring time in Lahore, with many fruitful discussions and opportunities for new contacts that will be of importance for the future of our field.

Best regards,

**Organizing Committee**

# PROCEEDINGS OF
# 4th INTERNATIONAL CONFERENCE

# ON

# CHEMISTRY (ICC) Hybrid Mode

**March 20-21, 2023**

**Compiled and Edited By:**

**Dr. Saz Muhammad and Mr. Muhammad Waqas**

**Organized by**

**Department of Chemistry**
**Lahore Garrison University**
**Lahore, Pakistan**
**http://icc.lgu.edu.pk**

# 4th International Conference on Chemistry (ICC-2023) Hybrid Mode: Modern Trends in Chemical, Biological and Material Sciences

**SCOPE OF THE EVENT:**

The conference offers the breadth and in-depth scope for students, researchers and industrial representatives to get in touch with worldwide research, innovations and developments in the fields of chemical, biological and material sciences. The advantage of this conference will be to explore and refresh knowledge through informative sessions and interactions with eminent researchers of the field. This will open up new horizons for future collaborations and industrial linkages.

**AIMS AND OBJECTIVES**:

This two day conference 4th in the series will bring together researchers from industry, academia and government and non-government organizations to discuss the state-of-the-art, and recent advancements in the field of chemical, biological and material sciences. The conference will be Gordon Conference style, with discussion sessions and panels, to allow extensive interactions among participants. The conference will address and harmonize the advancements in science and technology to achieve the sustainable development goals for uplift of education and research in developing countries.

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# Administrative Details of the Conference

**Patron-in-Chief**

Major General Shahzad Sikander, **HI (M),** (Retd)

Vice- Chancellor, Lahore Garrison University (**LGU)**

**Patron**

Brig Raheel Ashraf, **SI (M)** (Retd)

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**Co-Patron**

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**Conference Chair**

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**Conference Co-Chair**

Col Dr. Humayun Sattar**, SI (M) (**Retd)

Director Academics, Lahore Garrison University (**LGU**)

**Conference Focal Person**

Dr. Syeda Shaista Gillani

Chairperson, Department of Chemistry, Lahore Garrison University **(LGU)**

**Organizing Committee**

Dr. Manzar Zahra Awan **(Conference Secretary)**

Dr. Saz Muhammad **(Conference Joint Secretary)**

Mr. Muhammad Waqas (**Conference Coordinator)**

**Peer Review Committee**

Prof. Dr. Khalid Mohammad Khan (International Centre for Chemical and Biological Sciences H.E.J Karachi)

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Prof. Dr. Ahmed Adnan (Dean Basic Science GCU Lahore)

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Mr. Muhammad Waqas (Sr. Lecturer of Chemistry, **LGU**)

**Finance/ Registration Committee**

Dr. Farwa Batool (Assistant Professor of Chemistry **LGU)**

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Mr. Muhammad Waqas (Sr. Lecturer of Chemistry, **LGU**)

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Dr. Farwa Batool (Assistant Professor of Chemistry **LGU)**

**Moderator**

Dr. Sadaf Sarfraz (Assistant Professor of Chemistry **LGU**)

Dr. Affifa Tajammal (Assistant Professor of Chemistry **LGU**)

Dr. Iqra Zubair Awan (Assistant Professor of Chemistry **LGU)**

**Stage Coordinators**

Dr. Manzar Zahra (Assistant Professor of Chemistry **LGU**)

Dr. Farwa Batool (Assistant Professor of Chemistry **LGU)**

Mr. Muhammad Waqas (Senior Lecturer of Chemistry **LGU**)

**Media Committee**

Dr. Iqra Zubair Awan (Assistant Professor of Chemistry **LGU)**

Mr. Muhammad Ibrar (Assistant Lecturer of Chemistry **LGU)**

**Refreshment Committe**

Dr. Iqra Zubair Awan (Assistant Professor of Chemistry **LGU)**

Dr. Hammad Arshad (Assistant Professor of Biology, **LGU**)

Mr. Jigar Allah Ditta (Lecturer of Chemistry, **LGU**)

**Poster Session Coordinator**

Dr. Affifa Tajammal Member (Assistant Professor of Chemistry **LGU**)

**Discipline Committee**

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Mr. Muhammad Waqas (Senior Lecturer of Chemistry **LGU**)

Mr. Jigar Allah Ditta (Lecturer of Chemistry **LGU**)

Mr. Muhammad Ibrar (Student affairs Coordinator of Chemistry **LGU**)

CR’s & GR’s Of MPhil and BS Chemistry

**Technical Assistance Team**

Mr. Mubasher (IT team member)

Mr. Abbas (IT team member)

**Student Ambassador**

Garrison Chemical Society

# Program of

## 4th International Conference on Chemistry (ICC) 2023 Hybrid Mode

**Theme:**
**Modern Trends in Chemical, Biological and Material Sciences**

**March 20-21, 2023**


**Organized By:**

**Department of Chemistry, LGU, Lahore-Pakistan**

**http://icc.lgu.edu.pk**

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

# Day 1, Monday, March 20, 2023

## Opening ceremony 08:00 - 11:00

## Venue: Jinnah auditorium

**ICC-2023 is inviting you to a scheduled Zoom meeting.**
**Topic: ICC2023 OPENING CEREMONY DAY 1**
**Time: Mar 20, 2023 09:00 AM Islamabad, Karachi, Tashkent**
**Join Zoom Meeting**
**https://us06web.zoom.us/j/87243939664**
**Meeting ID: 872 4393 9664**

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|---|---|
| 08:30 | Registration |
| 10:00 | Arrival of the Chief Guest |
| 10:05 | Recitation of the Holy Quran |
| 10:10 | Nate e Rasool (PBUH) |
| 10:15 | Documentary LGU |
| 10:20 | Introductory remarks by **Dr. Benjamin E. Partridge,** Department of Chemistry, University of Rochester, Rochester, NY 14627, **USA** |
| 10: 30 | Welcome address by **Major General Shahzad Sikander (HI) M (Retd)**, Vice Chancellor, LGU |
| 10:40 | Address by the Chief Guest **Prof. Dr. Shahid Munir**, Chairperson, Punjab Higher Education Commission |
| 10:55 | Vote of thanks by **Dr. Syeda Shaista Gillani**, Chairperson Department of Chemistry, LGU |
| **Presentation of Souvenirs** | |
| **Tea break + Poster Presentation (11:00- 11:30)** | |

## LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode

March 20-21, 2023 Lahore Pakistan

**Day 1, Monday, March 20, 2023**

**Plenary Session 11:30 - 13:30**

**Venue: Jinnah Auditorium**

| **Session Chair-I Prof. Dr. Ahmad Adnan**<br>**Session Chair-II Prof. Dr. Ayesha Mohy ud Din** | **Session Chair-III Prof. Dr. Abdul Qadir**<br>**Session Chair-IV Prof. Dr. Munawar Ali Munawar** |
|---|---|
| **Moderator:**<br>Dr. Sadaf Sarfraz, Department of Chemistry, LGU, Lahore, Pakistan. | |
| **Plenary Lecture-I**<br>**Dr. Benjamin E. Partridge**<br>Assistant Professor, Department of Chemistry, University of Rochester, Rochester, NY 14627, **USA**<br>*Programming the Hierarchical Assembly of Biological and Bioinspired Molecules*<br>**11:30-12:00** | **Plenary Lecture -IV**<br>**Dr. Muhammad Saeed**<br>Associate Professor, Department of Chemistry, SBA School of Science and Engineering, **LUMS** Lahore<br>*Synthesis of Novel Hetrocyclic Compounds and Evaluation for Antiviral Potential*<br>**12:40-13:10** |
| **Plenary Lecture -II**<br>**Dr. Mariya-al Rashida**<br>Chairperson, Associate Professor, Department of Chemistry, **FCCU**, Lahore<br>*Therapeutic Potentials of Ectonucleotidase Inhibitors Derived from Chromones*<br>**12:00-12:20** | **Plenary Lecture -V**<br>**Dr. Muhammad Salman**<br>Associate Professor, School of Chemistry, University of the Punjab, Lahore<br>*Effective use of waste biomass after chemical modification for waste water metal detoxification*<br>**13:10 -13:30** |
| **Plenary Lecture -III**<br>**Dr. Nayab Batool**<br>Associate Professor, School of Chemistry, University of the Punjab, Lahore<br>*Trend of Thyroid dysfunction associated with visible Goiter*<br>**12:20-12:40** | |
| **Presentation of Souvenirs** | |
| **Lunch and Prayer Break (13:30- 14:00)** | |

**Day 1, Monday, March 20, 2023**

**Technical Session I & II 14:00 - 16:00**

**Venue: Iqbal Auditorium & Usman Shaukat Hall**

| **Technical Session I**<br>**Venue: Iqbal Auditorium** | **Technical Session II**<br>**Venue: Usman Shaukat Hall** |
|---|---|
| **Session Chair-I: Dr. Benjamin E. Partridge**<br>**Session Chair-II: Dr. Nayab Batool**<br>**Moderator:**<br>Dr. Farwa Batool, Department of Chemistry, LGU, | **Session Chair I: Dr. Mariya-al Rashida**<br>**Session Chair II: Dr. Muhammad Saeed**<br>**Moderator:**<br>Dr. Affifa Tajammal, Department of Chemistry, LGU, |

# LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode

March 20-21, 2023 Lahore Pakistan

| Lahore | Lahore |
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| **Oral Presenter-I**<br>**Dr. Shagufta Saeed**<br>Assistant Professor, Institute of Biochemistry and Biotechnology, UVAS, Lahore<br>*Valorization of locally available waste plant leaves for production of tannase and gallic acid by solid-state fermentation*<br>**14:00-14:15** | **Oral Presenter -IX**<br>**Dr. Saeed Ahmed**<br>Assistant Professor, HoD Dept. of Chemistry, University of Chakwal<br>*CTAB-assisted development of hierarchical flower-like multimorphology magnesium oxide for phosphate removal*<br>**14:00-14:15** |
| **Oral Presenter -II**<br>**Dr. Asma Ashraf**<br>Assistant Professor, Department of Zoology, Division of Science and Technology UE, Lahore, Pakistan<br>*Isolation and Characterization of Endomicrobes from the Hindgut of Microtermes obesi and their Plant Based Control*<br>**14:15-14:30** | **Oral Presenter-X**<br>**Dr. Hammad Arshad**<br>Assistant Professor, Department of Biology, Lahore Garrison University, Lahore.<br>*Green synthesized synthesis of silver nanoparticles and their antibacterial potential*<br>**14:15-14:30** |
| **Oral Presenter -III**<br>**Dr. Iqra Zubair Awan**<br>Dept. of Chemistry, LGU Lahore<br>*Oxalic Acid Medium for Metal Recovery from Layered Double Hydroxides Derived Mixed Oxides Catalysts*<br>**14:30-14:45** | **Oral Presenter-XI**<br>**Dr. Sidra Farid**<br>Assistant Professor, Department of Chemistry, Government College University Katcheri Road Lahore, Lahore<br>*Smart Textiles to Sniff out the Toxic Gases*<br>**14:30-14:45** |
| **Oral Presenter -IV**<br>**Dr. Ariba Farooq**<br>Assistant Professor, Dept. of Chemistry, University of Lahore<br>*Development of grapheme oxide loaded biocomposites films for controlled drug delivery and angiogenesis in wound healing.*<br>**14:45-15:00** | **Oral Presenter-XII**<br>**Ms. Hira Amjad**<br>Department of Chemistry, Government College University Katcheri Road Lahore, Lahore<br>*Synthesis, in vitro and in silico assessment of potential drug molecules having 3,5-disubstituted-1,2,4-triazole moiety. From scratch to bioactivities*<br>**14:45-15:00** |
| **Oral Presenter –V**<br>**Mr. Abdullah Shoaib**<br>School of Science Institute of Chemistry, UMT, Lahore<br>*Tailoring of Novel Empagliflozin Sodium Glucose co-transporter 2 (SGLT2) Inhibitor, Loaded Zinc Oxide Nanoparticles for Anti-Diabetic Activity*<br>**15:00-15:15** | **Oral Presenter -XIII**<br>**Ms. Rafia Imtiaz**<br>Department of Chemistry, GCU Lahore, Lahore<br>*Evaluation of Metal Foam Supported nanocomposites as electrocatalysts for Water Splitting*<br>**15:00-15:15** |
| **Oral Presenter -VI**<br>**Ms. Rabia Muazzam**<br>Govt. Queen Mary Graduate College, Lahore<br>*Lignin Activation and Vanillin Synthesis Using Plasma Assisted Ozone Reactor*<br>**15:15-15:30** | **Oral Presenter -XIV**<br>**Mr. Muhammad Salman Muhsan**<br>Department of Chemistry, GCU Lahore, Lahore<br>*Synthesis of bifunctional Cobalt Iron Borate catalyst for generation of hydrogen from alkaline sodium borohydride and Catalytic Applications in Reduction of 4-Nitrophenol* |

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| | **15:15-15:30** |
| **Oral Presenter -VII**<br>**Mr. Numan Ahmed**<br>Department of Chemistry, Zhejiang University, China<br>*Silsesquioxanes-Based Nanolubricant Additives with High Thermal Stability, Superhydrophobicity, and Self-cleaning Properties*<br>**15:30-15:45** | **Oral Presenter -XV**<br>**Mr. Sajid Hussain**<br>Dept. of Chemistry, UMT Lahore<br>*Development of Biochar Based Eletro Catalytic Material for Electrochemical Applications*<br>**15:30-15:45** |
| **Oral Presenter -VIII**<br>**Ms. Mamoona Riaz**<br>School of Science Institute of Chemistry, UMT, Lahore<br>Electrochemical $CO_2$ Reduction by Iron Porphyrin Complexes<br>**15:45-16:00** | |
| **Concluding Remarks and Souvenir Distribution by Session Chair (15:45- 16:00)** | **Concluding Remarks and Souvenir Distribution by Session Chair (15:45- 16:00)** |

**Day 2, Tuesday, March 21, 2023**

**Plenary Session (Online Session) 08:30 - 12:00**

**Venue: Jinnah Auditorium**

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| **ICC-2023 is inviting you to a scheduled Zoom meeting.**<br>**Topic: ICC2023 ONLINE TALK SESSION**<br>**Time: Mar 21, 2023 08:00 AM Islamabad, Karachi, Tashkent**<br>**Join Zoom Meeting**<br>**https://us06web.zoom.us/j/84227872614**<br>**Meeting ID: 842 2787 2614** | |
| **Session Chair-I Dr. Aisha Waheed Qureshi**<br>**Session Chair-II Dr. Muhammad Hafeez** | **Session Chair-III Dr. Syeda Shaista Gillani**<br>**Session Chair-IV Dr. Rahman Shah Zaib Saleem** |
| **Moderator:**<br>Dr. Farwa Batool, Department of Chemistry, LGU, Lahore, Pakistan. | |
| **Keynote Speaker-VII (online)**<br>**Professor Dr. Muhammad Sultan**<br>Department of Physics, Kohsar University, Murree Punjab, Pakistan<br>Emergence of Perovskite Solar Cells as Solution Processed Technology for Smart Energy Harvesting<br>**08:40-9:55** | **Keynote Speaker-V (online)**<br>**Dr. Shakeel Ahmad Shahid**<br>Deputy Local Safety Officer Switzerland & Liechtenstein<br>Chirality or Sidedness in Nature<br>**10:40-10:55** |

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

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| **Oral Presenter-XVI (Online)**<br>**Dr. Bilal Ahmad Khan**<br>Department of Chemistry, University of Azad Jammu and Kashmir, KAC, Muzaffarabad, 13100, AJK, Pakistan<br>*Synthesis and Evaluation of Novel S-alkyl phthalimide- and S-benzyl-oxadiazole-quinoline Hybrids as Inhibitors of Monoamine Oxidase and Acetylcholinesterase*<br>**9:55-10:05** | **Keynote Speaker-VI (online)**<br>**Prof. Dr. Abbas Khan**<br>Department of Chemistry, Abdul Wali Khan University, Mardan 23200, KPK, Pakistan<br>***Fabrication and Characterization of CuO-SiO2 Based Nanocomposites for Photocatalytic and Biological Applications***<br>**10:55-11:10** |
| **Keynote Speaker-II: (online)**<br>**Prof. Dr. Khalid Mohammed Khan**<br>H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan<br>*Synthesis of molecular hybrids as highly effective anti-leishmanial agents*<br>**10:05-10:20** | **Keynote Speaker-I (Online)**<br>**Prof. Dr. Jochen Bodem**<br>Institut für Virologie und Immunbiologie University of Würzburg, Germany<br>*The serotonin reuptake inhibitor Fluoxetine inhibits SARS-CoV-2 - characterization of the antiviral*<br>**11:10-11:25** |
| **Keynote Speaker-III (online)**<br>**Dr. Amanullah**<br>Associate Professor, Department of Chemistry, University of Alberta, Canada<br>*Efficient conversion of carbon dioxide ($CO_2$) and crude glycerol into value-added products*<br>**10:20-10:40** | **Keynote Speaker-VIII (online)**<br>**Dr. Atif Emre Demet**<br>**Department of Energy Systems Engineering, Necmettin Erbakan University, Konya, Turkiye**<br>*Modern Trends of Worldwide Active and Granted Lignin Patents*<br>**11:25-11:40** |
| **Keynote Speaker-IV (onsite)**<br>**Dr. Rahman Shah Zaib Saleem**<br>Associate Professor, Department of Chemistry, SBA School of Science and Engineering, LUMS Lahore<br>**11:40-11:50** | **Keynote Speaker-IX (online)**<br>**Prof. Dr. Francesco Di Renzo**<br>**ICGM, University of Montpelier-CNRS-ENSCM, Montpellier, France**<br>***Catalytic Hydrogen Transfer, Evaluation of an Alternate Tool for Redox Reaction***<br>**11:50-12:00** |
| **Presentation of Souvenirs** | |

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

**Day 2, Tuesday, March 21, 2023**

**Technical Session III & IV 12:00 - 13:30**

**Venue: Iqbal Auditorium & Usman Shaukat Hall**

| **Technical Session III**<br>**Venue: Iqbal Auditorium** | **Technical Session IV**<br>**Venue: Usman Shaukat Hall** |
|---|---|
| **Session Chair-I: Dr. Roheela Yasmin**<br>**Session Chair-II: Dr. Zeeshan Mustafa** | **Session Chair-I: Dr. Naureen Naeem**<br>**Session Chair-II: Dr. Syeda Mona Hassan** |
| **Moderator:**<br>Dr. Sadaf Sarfraz, Department of Chemistry, LGU, Lahore | **Moderator:**<br>Dr. Affifa Tajammal, Department of Chemistry, LGU, Lahore |
| **Oral Presenter -XVII**<br>**Dr. Sehrish Firyal**<br>Associate Professor, Institute of Molecular Biology and Biotechnology, University of Veterinary and Animal Sciences, Lahore-Pakistan<br>*Genetic Markers assisted selection of mastitis resistant dairy cattle*<br>**12:00-12:10** | **Oral Presenter -XXII**<br>**Dr. Zeeshan Mustafa**<br>Assistant Professor, Dept. of Physics, LGU Lahore<br>*Manipulation Exchange bias via Electric Field Driven Ion Implantation in All-Solid-State Li-Ion Redox Capacitor Structure*<br>**12:00-12:10** |
| **Oral Presenter -XVIII**<br>**Dr. Farwa Batool**<br>Assistant Professor, Dept. of Chemistry, LGU, Lahore<br>*Discovering Direct-Acting Antiviral Potential Drugs by Targeting NS2B/NS3 Dengue Virus Protease*<br>**12:10-12:20** | **Oral Speaker-XXIII**<br>**Ms. Noor Ul Huda**<br>Dept. of Chemistry, LUMS, Lahore<br>*Development of Silica-supported Catalysts for Depolymerization of Lignocellulosic Biomass via Lignin-first approach*<br>**12:10-12:20** |
| **Oral Speaker-XVIX**<br>**Ms. Ramsha Saleem**<br>Dept. of Chemistry, GC Lahore<br>*An Efficient Sponge like Ag2SnO3 Nanocatalyst for Selective Electroreduction of CO2 to Formate*<br>**12:20-12:30** | **Oral Presenter –XXIV**<br>**Ms. Shanza Rauf Khan**<br>Lecturer, Department of Chemistry, University of Agriculture, Faisalabad 38000, Pakistan<br>*Synthesis of Iron Sulfide Nanoparticles As Anti-Tick And Fuel Additive*<br>**12:20-12:30** |
| **Oral Presenter -XX**<br>**Mr. Ali Raza**<br>Dept. of Chemistry, University of Lahore, Lahore<br>*Molecular Modeling of Pyrrolo-Pyrimidine Based Analogs as Potential FGFR1 Inhibitors*<br>**12:30-12:40** | **Oral Presenter -XXV**<br>**Ms. Saleha Imran**<br>Dept of Chemistry, LCWU, Lahore<br>*Synthesis of Iron Oxide/Chitosan Nanocomposites – An Effective Approach Towards Environment Protection*<br>**12:30-12:40** |

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| **Oral Presenter-XXI**<br>**Dr. Saz Muhammad**<br>Assistant Professor, Department of Chemistry, LGU, Lahore<br>*Functional POSS based polyimide nanocomposite for enhanced structural, thermal, antifouling and antibacterial properties.*<br>**12:40-12:50** | |
| **Concluding Remarks and Souvenir Distribution (12:50- 13:00)** | **Concluding Remarks and Souvenir Distribution (12:50- 13:00)** |
| **Lunch Break (13:30- 14:00)** | |

**Day 2, Tuesday, March 21, 2023**

**Technical Session V & VI 14:00 - 15:00**

**Venue: Iqbal Auditorium & Usman Shaukat Hall**

| **Technical Session V**<br>**Venue: Iqbal Auditorium** | **Technical Session VI**<br>**Venue: Usman Shaukat** |
|---|---|
| **Session Chair-I: Dr. Muhammad Sarmad Arshad**<br>**Moderator**:<br>Dr. Affifa Tajammal, Department of Chemistry, LGU, Lahore | **Session Chair-I: Dr. Muhammad Hafeez**<br>**Moderator:**<br>Dr. Farwa Batool, Department of Chemistry, LGU, Lahore |
| **Oral Speaker-XXVI**<br>**Dr. Muhammad Tariq**<br>Associate Professor, Institute of Chemical Sciences, Bahauddin Zakariya University, Multan, Pakistan<br>*Synthesis, spectroscopic characterization, antimicrobial and DNA interaction studies of organotin(IV) carboxylates*<br>**14:00-14:15** | **Oral Speaker-XXIX**<br>**Dr. Sana Ahmad**<br>Associate Professor, Lahore College For Women University, Lahore<br>*Synthesis of Iron Oxide/Chitosan Nanocomposites – An Effective Approach Towards Environment Protection*<br>**14:00-14:15** |
| **Oral Speaker-XXVII**<br>**Mr. Ammar Hassan Jiskani**<br>Dept. of Chemistry, LUMS Lahore<br>*Expeditious Synthesis and Anti-viral Evaluation of 1,2,4-oxadiazoles against DENV NS2B/NS3Protease*<br>**14:15-14:30** | **Oral Speaker-XXX**<br>**Dr. Saima Naz**<br>Assistant Professor, Department of Chemistry, University of Education Lahore, Faisalabad Campus, 38000 Pakistan<br>*Ag doped β-SiC graphene nanoparticles with amplified electrical, Photocatalytic, and antibacterial activity: An accelerated flashing version.*<br>**14:15-14:30** |

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| **Oral Speaker-XXVIII**<br>**Ms. Sana Mansoor**<br>Research Associate, University of Management and Technology C-II, Johar Town, Lahore, Pakistan<br>*A facile method for the Nano Theranostics fabrication of composite CuO-GO-Ag; by using Fagonia arabica for the Antioxidant and Anti-Inflammatory Activity*<br>**14:30-14:45** | **Oral Speaker-XXXI**<br>**Mr. Masood Zafar**<br>Department of Chemistry, University of Education Lahore-Pakistan<br>*Facile synthesis of Polyaniline/Titania/CNTs based hybrid nanocomposites and their applications supercapacitors applications.*<br>**14:30-14:45** |
| **Concluding Remarks and Souvenir Distribution by Session Chair (14:45-15:00)** | |

**Day 2, Tuesday, March 21, 2023**

**Closing Ceremony 15:00 - 16:00**

**Venue: Jinnah Auditorium**

**ICC-2023 is inviting you to a scheduled Zoom meeting.**
**Topic: ICC2023 CONFERENCE CLOSING CEREMONY**
**Time: Mar 21, 2023 02:00 PM Islamabad, Karachi, Tashkent**
**Join Zoom Meeting**
**https://us06web.zoom.us/j/87024164406**
**Meeting ID: 870 2416 4406**

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|---|---|
| **15:00** | Arrival of Chief Guest |
| **15:05** | Recitation of the Holy Quran |
| **15:10** | LGU Documentary |
| **15:15** | Address by the Guest of honor **Dr. Shahzad Alam,** Former Chairman, PCSIR Islamabad |
| **15:20** | Address by the Guest of honor **Dr. Abdul Hafeez,** Director Pharmagen Limited |
| **15:25** | Address by the Chief Guest **Prof. Dr. Jamil Anwar,** Emeritus Professor, School of Chemistry, Former Pro Vice Chancellor, University of the Punjab, Former Vice chancellor Lahore Garrison University |
| **15:40** | Concluding Remarks by Conference Chair, **Col. Dr. Muhammad Amjad Khan (Retd)** Dean Basic science, LGU |
| **Presentation of Souvenirs, Tea and Group Photo** | |
| **Note:** The Conference program is final. Please ensure your attendance during the Conference by sending your confirmation email | |

# Keynote Lectures

K-01/ICC-04-23

## Programming the Hierarchical Assembly of Biological and Bioinspired Molecules

**Benjamin E. Partridge**

*Department of Chemistry, University of Rochester, Rochester, NY 14627, United States*

**Abstract:**

Nature achieves structural complexity in its materials through *hierarchical assembly*: a multistep process in which a series of assembly processes leads to a final materials state. This process—exemplified by the filamentation of actin and myosin to form muscle fibers—has emerged in natural systems as an efficient way to program functional structures across multiple length scales. Mimicking such hierarchy in synthetic materials is a grand challenge that, if met, will open the door to novel complex systems with functions that mimic, interface with, or even surpass those of natural systems. However, programming hierarchy into the self-organization of synthetic building blocks remains a significant challenge. In this presentation, I'll discuss recent and ongoing approaches towards meeting this challenge using foundational supramolecular chemistry, with particular emphasis on proteins, DNA, and synthetic DNA-like constructs.

K-02/ICC-04-23

## Efficient conversion of carbon dioxide ($CO_2$) and crude glycerol into value-added products

**Aman Ullah**

*Utilization of Lipids - Polymers/Materials Chemistry Group, University of Alberta, T6G 2P5 Canada*

**Abstract:**

Modern civilization has become dependent on fossil fuels as a source of energy and chemicals. As a result, the rapid industrial development and growing energy demand are pushing toward two imminent problems, the depletion of fossil fuel reserves and the negative impact on global climate. Subsequently, the lookout for renewable alternatives as energy sources and chemical feedstock has mobilized academia and industry to adapt

existing technologies and develop new methodologies. Biomass is currently the most widespread alternative feedstock due to its availability and relatively short regeneration cycle, yet its valorization has to deal with the waste those results from biomass processing. For instance, the biodiesel industry, the second larger biofuel manufacturer, generates approximately 10 wt. % of crude glycerol from the transesterification of vegetable oil, and 0.71 kg of $CO_2$ is released into the atmosphere per liter of biodiesel combusted as vehicle fuel. Thus, this presentation focuses on valorization routes for the major by-products from the biodiesel industry. We investigated the catalytic conversion of carbon dioxide ($CO_2$) to methanol, and a microwave-assisted rapid glycerol transformation to allyl monomers and polymers. The $CO_2$ was reduced to methanol in mini-batch reactors using a Cu/ZnO as an active phase supported on a novel hydrophobic material, phenyl polyhedral oligomeric silsesquioxane (POSS). Two types of POSS nanoparticles, octaphenyl POSS (O-POSS) and dodecaphenyl POSS (D-POSS) were compared to evaluate the influence of the cage size and the number of ligands in the $CO_2$ conversion and methanol yield. The nanoparticles had an average size of 7 nm (CuO/ZnO/O-POSS) and 15 nm (CuO/ZnO/DPOSS). The structural characterization of the as-synthetized materials revealed that CuO/ZnO were electron withdrawers from POSS. Furthermore, the increased number of phenyls attached to the siloxane cage augmented the catalytic system's hydrophobic character, resulting in higher $CO_2$ conversion and methanol yield under the conditions studied. Furthermore, we identified that the hydrophobic nature of the supports plays a decisive role in driving the reaction to completion. These conclusions emerged after comparing the results with Cu/ZnO supported on reduced graphene oxide (RGO). Although RGO had a higher surface area due to its hydrophilic character but yielded 0% of methanol under the conditions studied. The thermal gravimetric analysis revealed that the new catalytic systems were stable under the required temperature range (200 °C – 270 °C). Further, glycerol was converted to allyl alcohol through a formic acid-mediated metal-free deoxydehydration reaction under microwaves. The produced allyl alcohol was also converted to allyl formate and allyl phthalate. The synthesized monomers (allyl alcohol, allyl formate, and allyl phthalate) were polymerized using microwave-assisted polymerizations. The microwave-assisted method resulted in faster conversions and higher energy efficiency (>16 times less energy consumption)

compared to the conventional heating method to produce allyl alcohol. Overall, the ability to convert CO2 and glycerol into value-added products is undoubtedly an attractive concept from both an academic and an industrial point of view.

K-03/ICC-04-23

## The serotonin reuptake inhibitor Fluoxetine inhibits SARS-CoV-2 - characterization of the antiviral mechanism

**Jochen Bodem**

*Institut für Virologie und Immunbiologie University of Würzburg Verbacher Str. 7 97078 Würzburg Germany*

**Abstract:**

SARS-CoV-2 variants, such as the delta or omicron variants, with higher transmission rates, accelerated the global COVID-19 pandemic. Thus, novel therapeutic strategies need to be deployed. Recently, we reported the inhibition of SARS-CoV-2 by the serotonin reuptake inhibitor Fluoxetine. Later, others collected evidence that Fluoxetine suppressed the activity of the acid sphingomyelinase (ASM) by interfering with viral entry. Here, we described the acid ceramidase as the main target of fluoxetine. To discover these effects, we synthesized an ASM-independent fluoxetine derivative, AKS466. High-resolution SARS-CoV-2–RNA FISH and RTqPCR analyses demonstrate that AKS466 down-regulates viral gene expression. It is shown that SARS-CoV-2 deacidifies the lysosomal pH using the ORF3 protein. However, treatment with AKS466 or fluoxetine lowers the lysosomal pH. Our biochemical results show that AKS466 localizes to the endo-lysosomal replication compartments of infected cells, demonstrating the enrichment of the viral genomic, minus-stranded RNA and mRNAs there. Both fluoxetine and AKS466 inhibit the acid ceramidase activity, cause endo-lysosomal ceramide elevation, and interfere with viral replication. Furthermore, Ceranib-2, a specific acid ceramidase inhibitor, reduces SARS-CoV-2 replication and, most importantly, the exogenous supplementation of C6-ceramide interferes with viral replication. These results support the hypothesis that the acid ceramidase is a

SARS-CoV-2 host factor. Furthermore, we will provide evidence that cellular signaling cascades are involved in the ceramide-mediated change of the lysosomal pH.

K-04/ICC-04-23

## Synthesis of molecular hybrids as highly effective anti-leishmanial agents

**Khalid Mohammed Khan**

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

*Department of Clinical Pharmacy, Institute for Research and Medical Consultations (IRMC), Imam Abdulrahman Bin Faisal University, P. O. Box 31441, Dammam, Saudi* Arabia

**Abstract:**

Leishmaniasis is an infection that hit mainly the economically less stable class of people, widespread in 100 countries. Approximately 0.7-1 million additional cases of leishmaniasis per year are registered from almost 100 endemic countries. Leishmaniasis is a parasitic disease and exhibits four main clinical syndrome representations; cutaneous leishmaniasis (CL), mucocutaneous leishmaniasis (MCL), visceral leishmaniasis/kala-azar (VL), and post-kala-azar dermal leishmaniasis (PKDL). Nearly 90% of all VL cases occur in 3 endemic foci: **1**. India, Bangladesh, and Nepal; **2**. East Africa; and **3**. Brazil. Countless ground-breaking VL therapies have existed during the last 10-15 years but each exemplified serious deficiencies. Pentamidine and amphotericin B presented a second line of drugs, but these drugs have not experienced widespread practice due to the severe toxicities and economic in-viability. Added that no vaccine has been approved for human utilization to date. Consequently, there is an increasing demand for the development of new, low-priced, effective, and harmless drugs for the treatment of leishmaniasis. The design of newly developed antileishmanial agents is based on the concept of molecular hybridization. It is important to unlock the fact that molecular hybridization is a relatively newer idea in drug development that is based on the combination of pharmacophoric moieties of different bioactive molecules to produce a new hybrid structure. The concept has been effectively utilized in our group to develop structural motifs of various biological interests.

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

K-05/ICC-04-23

# New modulator of tubulin dynamics capable of overcoming multidrug resistance in cancer cells

**Rahman Shah Zaib Saleem**

*Department of Chemistry and Chemical Engineering, SBA School of Sciences and Engineering, Lahore University of Management Sciences, Lahore, 54792*

**Abstract:**

Microtubules are highly dynamic filamentous heterodimeric polymers that form spindle fibers during the process of mitosis and are one of the most validated cancer targets.[1] The success of drugs targeting microtubules, however, is often limited by the development of multidrug resistance.[2] Our group has been engaged in developing novel compounds that can display potent antiproliferative activities in cells of different origins and overcomes resistance to microtubule-targeting agents. In this regard, we report SSE15206 as a novel compound that can causes aberrant mitosis resulting in G2/M arrest due to incomplete spindle formation, a phenotype often associated with drugs that interfere with microtubule dynamics. SSE15206 inhibits microtubule polymerization both in biochemical and cellular assays by binding to colchicine site in tubulin as shown by docking and competition studies. Prolonged treatment of cells with the compound results in apoptotic cell death [increased Poly (ADP-ribose) polymerase cleavage and Annexin V/PI staining] accompanied by p53 induction. More importantly, we have demonstrated that SSE15206 is able to overcome resistance to chemotherapeutic drugs in different cancer cell lines including multidrug-resistant KB-V1 and A2780-Pac-Res cell lines overexpressing *MDR-1*, making it a promising hit for further studies to target multidrug resistance.

K-06/ICC-04-23

## Chirality or Sidedness in Nature

**Shakeel Ahmad Shahid**

*Deputy Local Safety Officer Switzerland & Liechtenstein Mepha Schweiz AG Basel, Switzerland*

**Abstract:**

The molecules of any element or compound, right spinning or left spinning, share exactly the same chemical and physical properties. What or who dictates their propensity to spin in any particular direction is a brain-twister enough, but when it comes to the most uncanny ability of life to detect which molecules are spinning in which direction, the question acquires bizarre astronomical proportions. None of the five senses bestowed to man are equipped with any known mechanism which an determine the spin of molecules. The spinning molecules leave no imprint on the property of matter to become detectable through human sensory organs“. In my talk I will share how mere opposite spin in same molecular compound of a medicine can play a disastrous role i.e. thalidomide disaster. The disaster which led to a totally new field of science „pharmacovigilance“, which is backbone of clinical trials during and after innovation of life saving drugs. Pharmacovigilance is the science and activities relating to the detection, assessment, understanding and prevention of adverse effects or any other medicine-related problem.

K-07/ICC-04-23

## Catalytic Hydrogen Transfer; Evaluation of an alternative tool for redox reactions

**Francesco Di Renzo**

*ICGM, University of Montpelier-CNRS-ENSCM, Montpellier, France*

**Abstract:**

Hydrogenation and hydrodeoxygenation reactions represent important tools for the sustainability of industrial chemistry. The replacement of oil-derived feedstocks with platform molecules from renewable resources requires coping with the oxygen content of

biomass, higher than the level needed for most target products. The use of renewable energy for production of molecular hydrogen by electrolysis is well developed and is introducing sustainable hydrogenation in several industrial processes. The use of reactive hydrogen from biomass-derived alcohol or glycol feedstocks provides an elegant alternative to electrocatalysis. The exchange of hydrogen between alcohol and carbonyl groups by the Meerwein–Ponndorf–Verley (MPV) reaction has allowed to replace noble metal catalysts in several specialty chemical productions. The realization that low molecular mass alcohols can generate active hydrogen by reforming in mild conditions has allowed to implement deeper hydrogenation reactions in the environment of organosolv processes. The use of bioalcohols formed in biorefineries as reagents for the controlled reduction of lignocellulosic feedstocks is at the basis of so-called lignin-based biorefineries. Hints for the choice between hydrogenation methods based on renewable energies or biobased feedstocks will be provided as the function of targeted processes.

# Invited Lectures

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

I-08/ICC-04-23

# Fabrication and Characterization of CuO-$SiO_2$ Based Nanocomposites for Photocatalytic and Biological Applications

**Abbas Khan**

*Department of Chemistry, Abdul Wali Khan University, Mardan 23200, KP, Pakistan*

**Abstract:**

Approximately 70-90% of the organism's body by mass is constituted by water and is highly important for their survival. Various chemical pollutants exist in the water which are introduced by various industries and have resulted in its contamination which directly affects the environment. Various approaches are in practice used to tackle these issues. Among these, semiconductor photocatalysis appears to be the cutting-edge technique for the degradation of wastewater contaminants.In this work, we are reporting the preparation, detailed characterization and photocatalytic degradation and biological activities of bimetallic oxides (CuO-$SiO_2$) nanocomposite. For this purpose, CuO, $SiO_2$ nanoparticles and CuO-$SiO_2$ nanocomposites were successfully synthesized through sol-gel process. The nanoparticles and nanocomposite were prepared by taking the $Cu(NO_3)_2.3H_2O$ as copper oxide precursor and TEOS as silica precursor using absolute ethanol and water as solvents The molar ratio of TEOS : Glycerol : $H_2O$ used was 1.5:1:6.6 respectively. The synthesized nanoparticles and nanocomposites were characterized by using Scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and Brunauer–Emmett–Teller (BET). The nanocomposites and individual nanoparticles were then applied as catalysts for their activities toward catalytic/photocatalytic degradation of crystal violet (CV) dye in an aqueous medium. The degradation progress was monitored by UV-Visible spectroscopic analysis. It was found that CuO-$SiO_2$ nanocomposite shows good photocatalytic activities toward removal of crystal violet dye as compared to the catalytic activities of its individual constitutes. The antileishmanial and antioxidant activities results indicate that synthesized materials have promising biological attributes.

I-09/ICC-04-23

# Synthesis of novel heterocyclic compounds and evaluation for antiviral potential

**Muhammad Saeed**

*Department of Chemistry and Chemical Engineering, SBA School of Science and Engineering, Lahore University of Management Sciences (LUMS), Lahore*

**Abstract:**

Dengue fever is a common viral infection that affects approximately 400 million peoples worldwide each year. Although the major dengue outbreaks in the recent history were confined to the tropical and subtropical countries, yet due to international travel, trade and global warming, the whole global population is under direct threat of future dengue outbreaks. There exists no specific antiviral drug or safe anti-Dengue vaccine for the treatment or prevention of Dengue infection. The virus is commonly transmitted in humans by the bite of infected *Aedes aegypty* mosquitos, which have found favourable abodes in several regions of Pakistan and thus pose a constant public health risk. This situation calls for a comprehensive research program for the discovery and development of anti-dengue therapeutics to curtail large scale pandemics in future. Drug repurposing/repositioning offers a great opportunity for expeditious identification and development of drugs with new targets. In this context, our research team has screened a commercial library (Selleck Chemicals), consisting of 1126 approved drugs or new molecule entities (NMEs) in advanced clinical trials. Using high throughput screening biochemical assay, we have identified 11 potent inhibitors of dengue virus protease. Interestingly, all the identified inhibitors possess similar heterocyclic scaffolds, indicating their unique potential to specifically bind to the dengue virus protease. Because of this and due to the fact that heterocyclic compounds have played a key role in imparting pharmacophoric properties in small organic molecules inspired us and many synthetic chemists to innovate, discover and develop simple and robust methods for the *de novo* construction of heterocyclic scaffolds. The fragment-size heterocyclic scaffolds (with MW $\leq$ 350), containing chemically diverse substituents could bind the target with high ligand efficiency, which would subsequently be

elaborated or merged to construct drug-like molecules with enhanced binding affinity to dengue protease and could result in the discovery of novel direct-acting anti-dengue therapeutics. In this presentation, I will highlight our most recent investigation on the syntheses of several libraries of benzothiophens, 1,2,4-oxadiazoles and 1,3-thiazolidin-4-ones and findings on the biological and biochemical screenings.

I-10/ICC-04-23

## Emergence of Perovskite Solar Cells as Solution Processed Technology for Smart Energy Harvesting

**Muhammad Sultan**

*Department of Physics, Kohsar University Murree, Pakistan*

**Abstract:**

The depleting fossil based energy sources and their devastating impact on environment leads it imperative to shift of energy dependence on renewable technologies. Si solar cells are dominant in today's market, however, there are several challenges associated with the use of Si technology at large scale for smart energy harvesting applications. Perovskite solar cells (PSCs) have recently emerged as novel solution processed technology, having potential to fulfill many contemporary requirements which cannot met by Si based solar cells. Enormous growth in the performance of PSCs up to 25% within one decade since their inception make them competitive technology for future. Degradation of halide perovskite materials upon ambient exposure is one of the major challenge for their commercial applications. Scientific community is working to address the challenges associated with PSCs to make them viable at large scale. Inorganic perovskite materials have emerged as potential candidate for stable perovskite optoelectronic applications in recent years owing to their appropriate bandgap and high thermal stability. However, the fabrication of high quality inorganic perovskite absorber layer is the main challenge to achieve highly efficient perovskite solar cells. In this talk I will discuss different strategies for the interfacial modification between absorber and charge transport layers. I will show how the growth control leads to substantial improvement in the performance of the device.

I-11/ICC-04-23

## Effective use of waste biomass after chemical modification for waste water metal detoxification

**Muhammad Salman**

*Center for Applied Chemistry, School of Chemistry, University of the Punjab*

**Abstract:**

In this study *Sorghum Bicolor (L)* is used in its raw and chemically modified form for the removal of metal ions form their aqueous solution(s). Raw and chemically altered biomass(s) are characterized using SEM, BET surface area, FTIR, Surface acidic and Basic groups and $pH_{pzc}$. Process parameters like Biomass dose, effect of time, initial concentration of metal ions etc. are optimized. Non-linear equilibrium and kinetic modelling is performed to evaluate the obtained results. The results are further used to investigate the metal attachment mechanism with biomass. Thermodynamic study is also performed to evaluate the change in enthalpy and entropy during the process.

I-12/ICC-04-23

## Therapeutic Potentials of Ectonucleotidase Inhibitors Derived from Chromones

**Mariya al-Rashida**

*Department of Chemistry, Forman Christian College (A Charterd University), Lahore*

**Abstract:**

Ectonulceotidases are a broad family of cell-surface located enzymes. They are responsible for hydrolysis of extracellular nucleotides and nucleosides, hence tightly regulating the availability of these nucleotides and their hydrolyzed products at their respective purinergic receptors. Together, these ectonucleotidases and purinergic receptors form the basis of the most diverse and ubiquitous nucleotide based cell-signaling system in the humans with vast therapeutic implications. Ectonucleotidases have four major types; i) nucleotide pyrophosphatase/phosphodiesterases (NPPs), ii) nucleoside triphosphate diphosphohydrolases (NTPDases), iii) ecto-5′-nucleotidase (e5'NT) and iv) alkaline phosphatases (APs or ALPs). Currently the lack of selective inhibitors of ectonucleotidsaes

is a considerable challenge in the further development of this field into transnational medicine. Our research group has synthesized several chromone based compounds and found them to be active inhibitors of ectonucleotidase enzymes. Some of the compounds were even found to be highly selective towards inhibiting a specific isozyme over others. Molecular docking studies provided insights into the nature of ligand interactions at the binding site, providing important clues regarding structural modifications that can lead to even better and possibly selective ectonucleotidase inhibition.

I-13/ICC-04-23

## Synthesis, Characterization and Antimicrobial Study of Copper (II) Complex with Ethyl-5-Hydroxy-2-Oxo-2H-Chromene-3-Carboxylate: X-ray analysis of [Cu (C 12 H 9 O 5 ) 2 .2H 2 O]

**Nayab Batool Rizvi**

*School of Chemistry, University of the Punjab Lahore, Pakistan*

**Abstract:**

A novel copper complex [Cu (C 12 H 9 O 5 ) 2 .2H 2 O] was synthesized by the reaction of copper salt (CuCl 2 .2H 2 O) and coumarin based ligand (Ethyl-5-hydroxy-2-oxo-2H chromene-3- carboxylate) at room temperature. The structure of complex under study was established by using various analytical techniques like melting point (M.P.), Infrared (IR) spectroscopy, Powder x-ray diffraction (PXRD), thermo gravimetric analysis (TGA), atomic absorption spectroscopy (AAS) and Mass spectrometry (ESI-MS). Ligand showed activity with MIC 15µg/ mL, 20µg/ mL, 40µg/ mL for *S. aurues, E. coli* and *S. typhi* respectively whereas MIC values of Cu-complex for above mentioned bacterial strains were found to be 10µg/ mL, 15µg/ mL, 20µg/ mL respectively. Ligand could not inhibit the growth of *p. auruginosa*, B. Subtilis, MRSA but Cu-complex showed MIC 10µg/ mL, 50µg/ mL for B. Subtilis and *p. auruginosa*. It also remained ineffective against MRSA.

# Oral Abstracts

O-14/ICC-04-23

# Valorization of Locally Available Waste Plant Leaves for Production of Tannase and Gallic Acid by Solid-State Fermentation

**Shagufta Saeed and Sehrish Firyal**

*Institute of Biochemistry and Biotechnology, University of veterinary and animal sciences, Lahore*

**Abstract:**

To evaluate the prospective of various indigenous plant leaves for biosynthesis of value-added products including tannase and gallic acid by *Aspergillus oryzae* FCBP-PTF-1202 in solid-state fermentation. Tannic acid-rich indigenous plant leaves *Psidium guajava* (guava), *Syzygium cumini* (black plum), *Eucalyptus globulus* (Eucalyptus), *Ficus benghalensis* (Banyan), *Citrus limon* (lemon), *Ficus religiosa* (Sacred fig), *Citrus sinensis* (Orange) and *Mangifera indica* (Mango) were analyzed to explore their potential as substrates for the production of tannase and gallic acid. After assessing all these substrates, black plum leaves produced the most promising effect resulting in a significantly ($p<0.05$) higher yield of tannase (138.34 U/g) and gallic acid (0.565 mg/g). Various influential physicochemical parameters were optimized to improve the yield of both end products. Results revealed that black plum leaves at a substrate water ratio of 1:2, pH 5.5, and temperature 30°C yielded the best production after 72 h of incubation period. Supplementation of glucose and nitrogen source to basal media increased the yield of tannase (179.95 U/g) and gallic acid (0.986 mg/g). Furthermore, the gallic acid produced was extracted by soxhlet apparatus and identified by Fourier-transform infrared spectroscopy FTIR. The purity of gallic acid produced was 98.5% as quantitatively analyzed by high performance liquid chromatography HPLC. In the end, production of tannase and gallic acid from plant leaves through the optimized environment via solid state fermentation can be exploited commercially to enhance our economy.

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

O-15/ICC-04-23

# Genetic Markers assisted selection of mastitis resistant dairy cattle

**Sehrish Firyal, Ali Raza Awan, Muhammad Tayyab, Shagufta Saeed, Rumisha Raza and Muhammad Wasim**

*Institute of Molecular Biology and Biotechnology, University of Veterinary and Animal Sciences, Lahore-Pakistan*

**Abstract:**

Cattle industry is one of the fast growing industries in dairy sector of Pakistan. This contributes 55.1 percent in value added GDP of agriculture and has remarkable potentials to expand. There are many economically important cattle breed of Pakistan. According to the field surveys of livestock diseases of Pakistan, mastitis is ranked as number one disease of our dairy animals. Mastitis is one of the shocking maladies of our dairy cattle causing production losses to our livestock industry. It negatively affects the milk production, quality of milk, and farm economics. Increasing the disease resistance among dairy animals is therefore desirable because without controlling this disease, the national goals to develop dairy farming on commercial and scientific lines as well as the production of wholesome milk which conforms to the standards of WTO Accord would remain elusive. It is very difficult to control this havoc plying disease because multiple environmental and genetic factors are involved in the development and progression of this disease. Susceptibility and resistance to mastitis is a complex trait influenced by genetic variation of animals. Among these variations, the polymorphisms in immunity genes are principal key factors in defensive mechanism of mammary gland. Current study has been designed to find the mastitis resistant and susceptible dairy Sahiwal cows. IL-8 gene was sequenced to find the resistant and susceptible genotype. This study would be helpful for animal breeders to proliferate the mastitis resistant genotype in dairy herds.

O-16/ICC-04-23

# Evaluation of Metal Foam Supported nanocomposites as electrocatalysts for Water Splitting

**Rafia Imtiaz, Muhammad Imran Abdullah, Muhammad Altaf, Raja Shahid Ashraf**

*Department of Chemistry, Government College University Katcheri Road Lahore, Lahore*

**Abstract:**

Electrocatalytic water splitting to generate clean and renewable fuels includes hydrogen using practical and attractive process of electrolysis of water. The occurrence of available energy reservoirs is decreasing steeply, therefore we are looking for an alternative and sustainable renewable energy resources [1]. It has been observed that a variety of ultra-durable, non-noble metal nanoparticles make effective electrocatalysts for hydrogen evolution reactions. In this work, nanocomposites on Ni foam is synthesized, which exhibits high and stable catalytic activity for both the OER and HER [2]. Herein, we present a one-step method to fabricate nanoparticles directly grown on Ni foam. The optimal catalyst only requires a small overpotential of 80 mV to drive 10 $mA.cm^{-2}$, and can provide a large current density of 800 mA $cm^{-2}$ at an overpotential of 660 mV for the OER. Moreover, it can afford 10 mA $cm^{-2}$ at an overpotential of 95 mV toward the HER. More importantly, this electrolyzer maintained its electrocatalytic activity even after continual water splitting for 20 h. This synthetic strategy has several advantages including facile preparation, low cost and can even be expanded to large-scale preparation for practical applications [3]. Overall, this methodology is one of the appropriate energy efficient ways to reduce the cost of water splitting devices, as it may simplify the diverse process and equipment.

O-17/ICC-04-23

## CTAB-assisted development of hierarchical flower-like multimorphology magnesium oxide for phosphate removal

**Saeed Ahmed**

*Department of Chemistry, University of Chakwal, Pakistan*

**Abstract:**

In this work, a series of hierarchical flower-like magnesium oxide (MgO) adsorbents were fabricated in a cetyltrimethylammonium bromide (CTAB) assisted solvothermal route using hexamethylenetetramine (HMTA) as a precipitating agent. Effects of CTAB feeding amount on the structure, morphology, pore structure, and corresponding adsorption behavior were investigated. The hierarchical gardenias flower-like MgO demonstrated a surface area of 336.54 m2g-1 at a minimum ratio of the CTAB/$Mg^{2+}$ in the reaction system. The hierarchical MgO phosphate removal capacity was found to be 265.11 mg g-1, which followed the pseudo-second-order and Freundlich isotherm model obtained from the large surface area and appropriate pore size. The value of n also suggesting the feasible nature of phosphate adsorption under the examined conditions. Indeed, this CTAB assisted hydrothermal method can provide a new understanding to tune the desired properties of a material by merely adjusting the reaction parameters.

O-18/ICC-04-23

## Synthesis of Iron Sulfide Nanoparticles as Anti-Tick and Fuel Additive

**Shanza Rauf Khan, Samra Jabeen and Sajid Ali**

*Department of Chemistry, University of Agriculture, Faisalabad 38000, Pakistan*

**Abstract:**

Current work is concerned with the morphology controlled synthesis of Iron sulfide (FeS) nanoparticles through wet chemical process. Three parallel reactions are conducted to obtain desired results. Crumb like aggregates having 10-100 nm size are obtained by using urea as a reducing agent and water as a solvent. Randomly oriented rod and cubic like particles having 20-120 nm size are obtained by using thiourea as sulfur source and water as a

solvent. The desired controlled morphology of Oval and spherical shaped FeS nanoparticles having 20-80 nm size are obtained by using ethylene glycol as organic solvent and PVP as stabilizer. Third reaction is conducted at basic pH through drop wise addition of $NH_4OH$. Sizes and morphologies of particles are obtained through STEM. EDX analysis confirmed the presence of iron and sulfur in the product. XRD data confirmed the amorphous nature of the product. Prepared iron sulfide nanoparticles are used as fuel additives and proved to be very useful in enhancing the fuel properties. Efficiency of fuel is analyzed at different dosage of FeS (20, 30, 40, 60 and 80 ppm). It is found that by increasing concentration of nanoparticles in fuel, the value of specific gravity increases and that of cloud and pour points, flash and fire points, kinematic viscosity, and surface tension decreases. Prepared FeS nanoparticles are coated with cypermethrin and deltamethrin to be used against ticks. Cypermethrin coated nanoparticles showed 100% mortality rate at 20, 25, and 30 mg/L concentration at 72 hours post exposure. 87% mortality rate was observed at 30 mg/L concentration after 24 hours of exposure. In case of deltamethrin coated nanoparticles, lower mortality rate was observed at each concentration as compared to that of cypermethrin.

O-19/ICC-04-23

## Green synthesized synthesis of silver nanoparticles and their antibacterial potential

**Hammad Arshad, Muhammad A. Sami, Saima Sadaf & Umer Hassan**

*Institute of Biochemistry and Biotechnology, University of the Punjab, Lahore, Pakistan*

*Department of Electrical and Computer Engineering, School of Engineering, Rutgers The State University of New Jersey, Piscataway, NJ, USA.*

*Global Health Institute, Rutgers The State University of New Jersey, New Brunswick, NJ, USA.*

*Department of Biology, Lahore Garrison University, Lahore, Pakistan*

**Abstract:**

Silver nanoparticles (AgNPs) exhibit strong antimicrobial properties against many pathogens. Traditionally employed chemical methods for AgNPs synthesis are toxic for the environment. Here, we report a quicker, simpler, and environmentally benign process to

synthesize AgNPs by using an aqueous 'root extract' of *Salvadora persica* (Sp) plant as a reducing agent. The synthesized *Salvadora persica* nano particles (SpNPs) showed significantly higher antimicrobial efficacy compared to earlier reported studies. We characterized SpNPs using UV–Vis spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Transmission Electron Microscopy (TEM), Field Emission Scanning Electron Microscopy (FE-SEM), Dynamic Light Scattering (DLS) and X-ray powder diffraction (P-XRD). UV–Vis spectrum showed the highest absorbance at 420 nm. FTIR analysis depicts presence of bond stretching including OH– (3300 $cm^{-1}$), C=N– (2100 $cm^{-1}$) and NH– (1630 $cm^{-1}$) which are attributed in the involvement of phenolics, proteins or nitrogenous compounds in reduction and stabilization of AgNPs. TEM, FE-SEM and DLS analysis revealed the spherical and rod nature of SpNPs and an average size of particles as 37.5 nm. XRD analysis showed the presence of the cubic structure of Ag which confirmed the synthesis of silver nanoparticles. To demonstrate antimicrobial efficacy, we evaluated SpNPs antimicrobial activity against two bacterial pathogens (*Escherichia coli* (ATCC 11229) and *Staphylococcus epidermidis* (ATCC 12228). SpNPs showed a significantly high inhibition for both pathogens and minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) were found to be 0.39 µg/mL and 0.78 µg/mL for *E. coli* while 0.19 µg/mL and 0.39 µg/mL for *S. epidermidis* respectively. Further, Syto16 staining of bacterial cells provided a supplemental confirmation of the antimicrobial efficacy as the bacterial cells treated with SpNPs stop to fluoresce compared to the untreated bacterial cells. Our highly potent SpNPs will likely have a great potential for many antimicrobial applications including wound healing, water purification, air filtering and other biomedical applications.

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

O-20/ICC-04-23

# Synthesis, in vitro and in silico assessment of potential drug molecules having 3,5-disubstituted-1,2,4-triazole moiety. From scratch to bioactivities.

**Hira Amjad, Dr Aziz Ur Rehman**

*Department of Chemistry, Government College University, Lahore*

**Abstract:**

The pandemic problem and growth of anti-biotic resistive microbes persuade us to synthesize broad spectrum novel anti-biotics that create a huge change in the field of medicines. The synthesis of novel compounds in given research is an effort to provide better medicinal specie for the benefit of mankind not only in terms of health but also economically and least side effects. In this work, heterocycles such as piperidine along with famous 1,2,4 triazole moiety has been used for structure activity relationship study along with the biological activities to find their probability to use as drugs. The different derivatives were based upon range of alkyl and aryl halides. The whole series of compounds was synthesized from a simple piperidine-4- carboxylate and 4-chlorobenzene sulfonyl chloride to 5-{1-[(4-chlorophenyl)sulfonyl]-4-piperidinyl}-4-ethyl-4H-1,2,4-triazol-3-thiol using multi-step synthesis which were characterized by FTIR, $^{1}$HNMR, $^{13}$CNMR and EIMS. The anti-bacterial activity was observed using biofilm inhibition which resulted in better activity against the gram-positive bacteria while the hemolytic activity was also observed which also claims about the toxicity of compounds. The series of compounds were analyzed against three different enzymes named urease, acetyl cholinesterase (AChE) and butyryl cholinesterase (BChE) enzyme. It was observed that the compounds having benzyl substitution had the better activities against the enzymes. The computational studies also confirmed the results from the enzyme activities while physicochemical properties and ADMET was also observed using the same. The in-silico studies proved many compounds to be potentially drug, non-toxic and least side effects.

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

March 20-21, 2023 Lahore Pakistan

O-21/ICC-04-23

# Isolation and Characterization of Endomicrobes from the Hindgut of *Microtermes obesi* and their Plant Based Control

**Asma Ashraf**

*Department of Zoology, Division of Science and Technology, University of Education, Lahore, Pakistan*

**Abstract:**

In the present investigation five bacterial species were isolated from the gut of *Microtermes obesi.* These isolates were characterized by Gram staining, biochemical tests and further phylogenetic analysis was carried out by using 16S rRNA. Gram reaction results showed gram negative cocci, bacilli and gram positive bacilli. Phylogenetic analysis confirmed *Paracoccus yeeii, Candidatus azobacteroides* and 2 species of *Candidatus endomicrobium.* Growth inhibitory effect of *G. robusta, E. camaldulensis, O. basilicum, C. papaya* and *E. globulus* was evaluated by agar well diffusion method. Plants were extracted by Soxhlet extraction apparatus and different concentrations (100, 500, 1000, 1500 and 2000ppm) were prepared. Maximum zone of inhibition was shown by *E. globulus* with 5.66mm at maximum concentration for isolate 5 whereas the minimum effectiveness was observed for *O. basilicum* with 0.90mm zone of inhibition at 2000ppm for *Paracoccus yeeii*. Plants effectiveness was as *E. globules>E. camaldulensis>G. robusta>O. basilicum >C. papaya*. The study concluded that the use of medicinal plants could be an alternative way to check bacterial growth and indirectly control termite infestation.

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

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O-22/ICC-04-23

# Molecular Modeling of Pyrrolo-Pyrimidine Based Analogs as Potential FGFR1 Inhibitors

**Ali Raza**

*Department of Chemistry, University of Lahore*

**Abstract:**

Fibroblast growth factor receptors 1 (FGFR1) is an emerging target for the development of anticancer drugs. The hyper-activation and uncontrolled expression of FGFR 1 are strongly associated with a number of different types of cancer. Apart from a few FGFR inhibitors, the members of the FGFR family have not been adequately investigated to develop clinically effective anticancer medicines. The use of proper computational approaches may aid in the deeper understanding of the foundations of protein–ligand complex formation, providing a better concept for building potential FGFR1 inhibitors. In this study, a variety of computational techniques, including 3D-QSAR, flexible docking and MD simulation followed by MMGB/PBSA, H-bonds and distance studies has been employed to systematically explore the binding mechanism of pyrrolopyrimidine derivatives against FGFR1. The 3D-QSAR model generated to deduce the structural determinants of FGFR1 inhibition. The high q2 and r2 values for the CoMFA and CoMSIA models indicated that the created 3D-QSAR models could reliably predict the bioactivities of FGFR1 inhibitors. The computed binding free energies (MMGB/PBSA) for the selected compounds were consistent with the ranking of their experimental binding affinities against FGFR1. We also conducted per-residue energy decomposition analysis to identify the key amino acids predominantly facilitating the ligand binding. The results indicated that the residues Lys514, Asn568, Glu571, and Asp641 of FGFR1 exhibited a strong tendency to mediate ligand-protein interactions through the hydrogen bond (H-bond) and *van der Waals* (*vdW*) interaction with FGFR1 inhibitors. These findings may aid researchers in better understanding the mechanism of FGFR1 inhibition and may serve as a guideline for developing novel potent FGFR1 inhibitors.

O-23/ICC-04-23

## Synthesis, Spectroscopic Characterization, Antimicrobial And Dna Interaction Studies Of Organotin(IV) Carboxylates

**Rabbia Khan, Muhammad Tariq, Hafiz Muhamamd Asif, Muhammad Ali Khan**

*Division of Inorganic Chemistry, Institute of Chemical Sciences, Bahauddin Zakariya University, 60800-Multan, Pakistan*

**Abstract:**

Six organotin(IV) carboxylates based on oxygen donor ligand have been synthesized and characterized by elemental analysis, FT-IR, NMR ($^{1}$H, $^{13}$C) and single crystal X-ray analysis. The bidentate mode of coordination of ligand with organotin(IV) moiety was observed leading to octahedral and trigonal bipyramid geometry. The complexes were screened for antimicrobial, cytotoxicity and anti-tumor activities. The results showed significant activity in each area of the activity with few exceptions. DNA interactions studies of ligand **HL** and their complexes were investigated by UV-Vis absorption spectroscopy and viscosity measurements. The results showed that both ligand **HL** and complexes interact with SS-DNA *via* intercalation as well as minor groove binding.

O-24/ICC-04-23

## A facile method for the Nano Theranostics fabrication of composite CuO-GO-Ag; by using *Fagonia arabica* for the Antioxidant and Anti-Inflammatory Activity

**Sana Mansoor, Sammia Shahid**

*Department of Chemistry, School of Science, University of Management and Technology, CII Johar Town, Lahore-54770, Pakistan*

**Abstract:**

In the present research work, CuO-GO-Ag nanocomposite was synthesized by using plant extract of *Fagonia arabica*, a medicinal herb. Copper Oxide nanoparticles (CuO NPs) and silver nanoparticles (Ag Nps) were prepared by the biological method. Graphene Oxide

was synthesized by commonly reported hummer's methods (with some changes) and hydrothermal approach. The characterization techniques to confirm the successful formation of our desired nanocomposite include SEM, XRD, EDX, and UV-Visible spectroscopy. The green synthesized CuO nanoparticles were firstly assorted with graphene oxide (GO) followed by the incorporation of silver nanoparticles. The antioxidant and anti-inflammatory potential of Nanocomposite was investigated. The nanocomposite capacity to reduce inflammation and protect against free radicals was assessed by using UV-Visible spectroscopy. According to the findings, biologically produced CuO- GO-Ag NCs have a strong potential for scavenging and reducing inflammation. To check the efficiency the results obtained from the fabricated nanocomposite were compared with standard ascorbic acid and diclofenac sodium. CuO-GO-Ag results revealed that the standard (ascorbic acid) had scavenging efficiencies of 44.22% for 0.3 mg/ml and 58.42% for 0.5 mg/ml, compared to 57.40% and 74.24% respectively. Similarly, diclofenac sodium showed a percentage inhibition of about 10.98 and 35.37 at a similar concentration, while CuO-GO-Ag nanocomposite showed a percentage inhibition of 46.59 and 87.80 at 0.1 mg/ml and 0.5 mg/ml.

O-25/ICC-04-23

## Smart Textiles to Sniff out the Toxic Gases

**Sidra Farid**

*Department of Chemistry, Government College University Lahore*

**Abstract:**

This work described the conversion of zero-valent copper metal to conductive two dimensional (2D) bimetallic Nickel pthalocyanine based metal–organic framework (NiPc-Cu-O) by a novel method of Oxidative Restructuring. This innovative method enables patterning of MOF onto a variety of flexible and porous substrates (cotton, silk, weigh paper, filter paper, nylon, Nyco, army fabric, cotton pant, polyester and conductive Carbon paper) with high resolution (500 µm) without any specialized equipment. This method produces electronic textiles with sheet resistances of 0.02–30 MΩ/cm$^2$ and uniform conformal coatings of MOF on textile swatches with strong interfacial contact capable

of withstanding chemical and physical stresses. These functional e-textiles were used to sniff the toxic gases i.e. $NH_3$, CO, NO and $H_2S$. These wearable chemiresistive sensors not only sense these nasty gases but also able to decontaminate them and be explored further in environmental remediation.

O-26/ICC-04-23

## Synthesis of β-SiC/$TiO_2$ hybrid via solid state method: Influence of graphene contact on electrical properties of β-SiC/$TiO_2$ hybrid

**Saima Naz**

*Department of Chemistry, University of Education Lahore, Faisalabad Campus, Pakistan*

**Abstract:**

The composition of hybrid materials is a recent trend to explore the materials properties for various advanced technological applications that are designed primarily on basis of the band alignment. It is necessary to develop such kind of materials for energy applications in order to find a suitable candidate for commercial viability. 3C-SiC/$TiO_2$ is one of the hybrid compositions that is considered as suitable candidate for various photovoltaic and photocatalytic applications. We have successfully synthesized 3C-SiC/$TiO_2$ hybrid material by simple route of solid state reaction and characterized by XRD, SEM, FTIR, Raman spectroscopy and UV-visible spectroscopy. The IV measurements of all grown samples by this method with a graphene contact show higher conductivity compared to the samples grown by complex and advanced growth techniques. The enhanced performance of synthesized hybrid material may be attributed to the proper band edge potentials that is the prerequisite condition for photovoltaic applications.

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O-27/ICC-04-23

# Facile synthesis of Polyaniline/Titania/CNTs based hybrid nanocomposites and their applications supercapacitors applications

**M Masood Zafar, Dr. Amina Asghar, Dr. Sumaira Nosheen**

*Solid State Physics Department, Punjab University and University of Education, Lahore*

**Abstract:**

In this study, $TiO_2$/PANI/CNTs hybrid polymer-metal nanocomposites were synthesized and their potential applications were explored intensively in portable energy storage devices mainly supercapacitors. Nanocomposites synthesis was carried out via oxidative in-situ polymerization route. Polymer properties were improved by varying the %age concentrations of titanium dioxide and carbon nanotubes as filler materials. Moreover, Carbon Nanotubes were also synthesized using graphite following chemical route. Various structural and morphological features of nanocomposites were characterized using FT-IR spectroscopy, XRD and SEM techniques. Optical microscopy was done to study the surface topography of nanocomposites using visible light and high magnification lenses. Material strength and deformation behavior was also investigated by compression testing with excellency at 8011.63. Hardness was tested to check the suitability of polymer nanocomposites with outstanding value of 95.5 with shore A. Electrical conductivity of nanocomposites was enhanced by treating with epoxy matrix. Maximum electrical conductivity achieved by nanocomposites was $12.5x10^{-2}$S/m manifesting highly resistive nature with epoxy resin. Additionally, stress and strain behavior of samples was examined with respect to time. Electrochemical measurements such as CV, GCD, EIS, and supercapattery performance were investigated in three and two cell configurations. These nanocomposites were used as positive electrode material in an asymmetric device and activated carbon was employed as negative electrode material. Battery-grade as well as capacitive material was combined utilized in a single device. Among a series of synthesized nanocomposites, an excellent performance was delivered via PANI/1%$TiO_2$/0.5%CNTs which lead to specific capacity and specific capacitance of 781 and 1302, respectively at scan rate of 1mV/s and galvanostatic charge-discharge of 678sec at 1A/g. The exceptional mechanical properties along with outstanding electrochemical performance made

PANI/1%$TiO_2$/0.5%CNTs valuable electrode material for development of advance storage supercapettery devices.

O-28/ICC-04-23

## Synthesis of Iron Oxide/Chitosan Nanocomposites–An Effective Approach Towards Environment Protection

**Sana Ahmad, Ayesha Saman, Saleha Imran**

*Lahore College for Women University, Lahore*

**Abstract:**

The research work comprised of synthesis of $Fe_3O_4$/Chitosan nanocomposites for the removal of water pollutants. $Fe_3O_4$ nanoparticles were synthesized by coprecipitation method and then sol-gel method was used to prepare $Fe_3O_4$/Chitosan nanocomposites. The nanocomposites were prepared in different weight ratios i.e. 1:1, 4:1, 8:1 and the magnetic nature of the nanocomposites caused easy separation from the solution by using an external magnet. The prepared nanocomposites were characterized by using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction analysis (XRD) and Scanning electron microscopy (SEM). The synthesized nanocomposites were used for the removal of atrazine pesticide from the aqueous solutions. The influence of different parameters such as time of contact between the nanocomposites and the pesticide, pH of medium and concentration of nanocomposites was also studied. Results showed that $Fe_3O_4$/Chitosan (8:1) nanocomposites were the excellent adsorbent out of all the three nanocomposites prepared. Up to 98% atrazine pesticide was removed at 6 pH in 120 min. Kinetic study indicated that the adsorption process is 1st order.

O-29/ICC-04-23

## Development of Silica-supported Catalysts for Depolymerization of Lignocellulosic Biomass via Lignin-first approach

**Noor Ul Huda**

*Lahore University of Management Sciences*

**Abstract:**

About 95% of the carbon-containing chemicals that sustain our daily lives are obtained from crude oil. Rapid depletion of crude oil supplies and escalating environmental effects of fossil resource utilization have led to the current strong drive, widespread interest, and investments in renewable resources to synthesize chemicals. Biomass is the only renewable carbon resource to derive both fuels and chemicals among various available substitutes. Lignocellulose is the most abundant form and, being inedible biomass, will not impose a direct negative impact on food supplies. Therefore, it serves as an ideal feedstock for replacing fossil resources in producing functional chemicals. Lignocellulosic biomass primarily consists of lignin and carbohydrates (cellulose and hemicellulose). The latter has been extensively studied and observed to be a versatile feedstock for the production of fuels and chemicals. However, the efficacy of lignin—the largest source of natural aromatics—is still untapped due to its high recalcitrant nature and complex structure. Efficient lignin depolymerization with an effective catalytic system followed

O-30/ICC-04-23

## Tailoring of Novel Empagliflozin Sodium Glucose co-transporter 2 (SGLT2) Inhibitor, Loaded Zinc Oxide Nanoparticles for Anti-Diabetic Activity

**Abdullah Shoaib, Sammia Shahid,**

*Department of Chemistry, School of Science, University of Management and Technology, CII, Johar Town, Lahore, Pakistan*

**Abstract:**

Empagliflozin was an inhibitor of sodium-glucose co-transporter-2 and used in the management and treatment of diabetes mellitus type-2. In the present study Zinc Oxide

nanoparticles were prepared by the chemical co-precipitation method and tailored with the novel Empagliflozin drug by the surface physio-sorption method and evaluated by the HPLC method, as the 59.76 percent of the drug was tailored. The tailored product was characterized as Ultravoilet-visible spectroscopy confirmed the generation of zinc oxide nanoparticles as the absorption spectra showed absorption maxima at 365 nm, Fourier transform Infrared showed at wave numbers between 430 and 445 $cm^{-1}$ in the composite confirming the tailoring of the zinc oxide nanoparticles with the drug. The XRD analysis determination of the crystallite's size resulted in 12.35 nm. Scanning electron microscope showed mono-dispersion of nanoparticles and a sphere-like shape, with the average particle size of which is 17 nm whereas the elemental analysis with the energy dispersive X-ray showed the sharp peaks of the Zinc and Oxygen. Further, the Freundlich isotherm model best explained the data for physio-sorption study. The in-vitro antidiabetic assays with enzymes α-amylase, and α-glucosidase were performed and it was studied that the composite showed the highest 81.72 and 92.77 percent inhibition of α-amylase and α-glucosidase at 1000 µg/ml concentration with the $IC_{50}$ value 3.06 and 72.44 µg/mL respectively showing the maximum and improved antidiabetic activity.

O-31/ICC-04-23

## An Efficient Sponge like $Ag_2SnO_3$ Nanocatalyst for Selective Electroreduction of $CO_2$ to Formate

**Ramsha Saleem1, Dr. Rana Rashad Mahmood Khan1, Dr. Zohaib Saeed**

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

**Abstract:**

The $Ag_2SnO_3$ nanoparticles were prepared by simple and cost-effective chemical reduction method. The as-synthesized nanocatalyst was employed to reduce $CO_2$ electrochemically in an aqueous electrolyte media at pH 6.8 using H-type cell. The catalyst looks like a sponge. The electrochemical results show higher current density (26 mA/cm2) and FE, long term stability, and product selectivity on the electrode. The highest FE for formate was 89% at -1.3 V *vs.* Ag/AgCl. The FE was found high as compared to monometallic (Ag, Sn) nanoparticles that indicate the synergistic effect between these metals.

O-32/ICC-04-23

# Development of grapheme oxide loaded biocomposites films for controlled drug delivery and angiogenesis in wound healing

**Ariba Farooq**

*Department of Chemistry, The University of Lahore, Lahore, Pakistan*

**Abstract:**

Graphene has got much attention in recent years and is considered one of the most promising nanomaterials because of its exceptional properties and applications. This research paper demonstrates the efficacy of graphene oxide (GO) on chitosan based polymeric system for their angiogenesis and controlled drug delivery potential. The dressings were prepared by casting method. A series of films/hydrogels were fabricated (with and without graphene oxide). Swelling indices of prepared hydrogel samples were determined in different media including distilled water, different pH and electrolyte solutions. The sample with best swelling was selected for loading of graphene oxide and drug delivery application. Scanning electron microscopy (SEM) was utilized to check the surface morphology and Fourier transform infra-red spectroscopy (FTIR) investigated chemical structures. We related the discharge/release phenomenon of medicines in test samples simultaneously. Antimicrobial tests showed materials were non-toxic and chorioallantoic membranes assay (CAM) confirmed that the GO loaded chitosan stimulated angiogenesis much higher than sample without GO dressings. Addition of GO enhanced its properties not only for the purpose of control drug delivery but also promoted angiogenesis and thus these materials can be used as a potential candidate for the wound dressings.

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O-33/ICC-04-23

# Silsesquioxanes-Based Nanolubricant Additives with High Thermal Stability, Superhydrophobicity, and Self-cleaning Properties

**Numan Ahmed, Hong Fan**

*State Key Laboratory of Chemical Engineering, College of Chemical and Biological Engineering, Zhejiang University, Zheda Road no. 38, Xihu District, Hangzhou 310027, China*

**Abstract:**

Nano additives are promising materials for long-envisioned next-generation lubricants to achieve excellent tribological performance and thermal stability. Here, an instigative and novel approach has been scrutinized to facilely prepare the nanolubricant additive. For this purpose, three synthetic strategies were designed for i) preparation of uniform-sized poly(methyl silsesquioxane) (PMSQ) nanoparticles, ii) hydrosilylation of the long carbon chain of ethyl 10-undecenoate and iii) modification of PMSQ nanoparticles with hydrosilylation product through a condensation reaction, in order to obtain long-carbon-chain grafted nanohybrids. The morphology, composition, and properties of these nanohybrids were confirmed by 1H-NMR, FTIR, SEM, EDS, and TGA. The effects of different concentrations of unmodified and modified PMSQ nanoparticles on the tribological properties of silicone oil were discussed. In the comparison of unmodified PMSQ nanoparticles, the modified one performs very well to reduce the coefficient of friction and wear scar diameter at low concentration. The TGA results revealed the extraordinary thermal stability of these particles, as their weight loss was only 19% at 800 °C which is remarkably higher than other solid lubricant additives. In this research, we tried to fill the deficiency of thermally stable material in the field of heavy machinery and industry. In addition, the environment-friendly (fluorine-free), superhydrophobic and self-cleaning surface effect of modified PMSQ nanoparticles was also observed. These silsesquioxane-based nanohybrids having synergistic effects, advantageous scientific values, and promising application prospects are expected to be more useful with other longer carbon chains.

O-34/ICC-04-23

# Expeditious Synthesis and Anti-viral Evaluation of 1,2,4-oxadiazoles against DENV NS2B/NS3 protease

**Ammar Hassan Jiskani and Muhammad Saeed**

*Department of Chemistry and Chemical Engineering LUMS, Lahore Pakistan*

**Abstract:**

Flaviviruses are tiny, enclosed animal viruses, having a single stranded genomic RNA. The pathogenic function of mosquito-borne flaviviruses in the disease development of Yellow Fever, Dengue Fever, and Zika Fever is critical. Vaccination has had minimal success in the prevention of flavivirus-related diseases thus far; therefore, concurrent efforts are required to develop direct-acting anti-viral (DAA) medications to combat these diseases. In this context, the flaviviral non-structural-3 (NS3) protein, in association with its cofactor non-structural-2B (NS2B), has emerged as a key target for DAA medication development. The complex NS2B/NS3 has proteolytic activity and catalyses co- and post-translational changes of the flaviviral polyprotein, making it a key viral replication factor. Our goal is to identify new DAA medicines against DENV and ZIKV infections by targeting the NS2B/NS3 protease complex encoded by the dengue virus (DENV) and Zika virus (ZIKV). Well-known pharmacological drugs that include the 1,2,4-oxadiazole skeleton have demonstrated interesting biological properties such as antivirals, adenosine receptor antagonists, antimicrobials, immunostimulatory medicines, anti-cancer agents, and anti-diabetic medications. Our goal in this research was to determine how effective ODZs would be against the flavivirus NS2B/NS3 protease. Thus, we have synthesized a library of sulfonamide-containing ODZs and used an in-house developed protease assay to determine their inhibitory potential against DENV NS2B/NS3. To further understand atomic level details of interaction between protease and inhibitor we have conducted computational modelling, which have pointed out the binding at the active side of the protease. The discovered DENV protease inhibitors have the potential to become novel DAA medicines for the treatment of DENV infections.

# Poster Abstracts

P-35/ICC-04-23

# Antibiofilm Potential of Nanoparticles Synthesized From Phytochemicals to Control Eye Infections Related To Contact Lenses

**Hirra Sajjad and Aisha Waheed Qurashi,**

*Department Of Biology, Lahore Garrison University Sector C Phase 6 DHA Lahore*

**Abstract:**

Contact lenses are extensively used However, major cause of eye discomfort (burning, drying, itching, irritation) and ocular infections such as contact lens-related acute red eye (CLARE), contact lens peripheral ulcer (CLPU), and fungal and bacterial keratitis by fungi (*Aspergillus*, *fusarium*, and *candida)* and bacteria (*Staphylococcus aureus* (Gram-positive), *pseudomonas aeroginosa* (Gram-negative) and also multi-drug resistant bacteria (*Serratia marcescens*. Quick diagnosis and treatments are needed to ensure the care of the eye and for preventing resistance among microbes to medicines. Use of natural products is desired like phytochemicals based nanoparticles. These are used as the nanocoating showing hydrophilic nature, low cost, and long-lasting superior cytocompatibility. Many plant based chemicals, like leaves extract of oregano (*origanum Vulgare*), and Fermented extracts of garlic (*Allium sativum*) exhibits antimicrobial and antibiofilm property for the prevention of eye infections. That is why it is a good side of interest to protect eye health by using natural plant-based products having no/fewer side effects. The present study has described the foundations for the development of products safe for the eyes while overcoming biofilm formation in future medicine.

**LGU 2023 – 4th International Conference on Chemistry (ICC) Hybrid Mode**

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P-36/ICC-04-23

# A Convergent Synthesis Of The Pyrazolone Based Hetarylidenes As New Antioxidant Agents

**Farah Iqbal, Faryal Chaudhry, Sijal Dar, Uswa Farooq**

*Department of Chemistry, Kinnaird College for Women, 93-Jail Road, Lahore-54000, Pakistan*

## Abstract:

The accumulation of free radicals can damage the cells which may instigate dangerous diseases in human beings. Therefore, contribution of antioxidants in scavenging or minimizing the impacts of such free radicals is of great significance. Different research studies have claimed that heterocyclic nuclei are the core elements in the structural frameworks of many potent antioxidant pharmacophores. In this context, the present study was thus designed in which an ultrasound mediated facile synthetic approach was adopted to prepare some hetarylidenes 3(a-h) engineered with the pyrazolone motif followed by the preliminary in vitro evaluation of radical scavenging potentials of these synthesized scaffolds. The sonication process assisted this condensation reaction very well and improved the results both in terms of product yields (up to 92%) as well as in reaction times (45-60 min) in comparison with our prior findings. Afterwards, the synthesized derivatives were screened out for their antioxidant potentials against DPPH free radical. Overall, this series displayed moderate to good free radical scavenging activity. The observed structure-antioxidant activity relationship could be considered for further in-depth investigations.

P-37/ICC-04-23

## Nanoparticle-based therapeutic approaches for wound healing

**Aleena Zainab, Aleesha Naheed, and Hammad Arshad**

*Department of Biology, Lahore Garrison University, Lahore*

**Abstract:**

Wound healing is a complicated anatomical procedure and is challenging. As reported, many coexisting diseases (diabetes, vascular diseases, etc.) significantly impact wound healing. Factors like repetitive injury, age, or hypertrophic scarring also affect wound healing. During the last years, the improvement of wound dressing biomaterials has registered a new standard level and superior knowledge based on chronic wound pathogenesis has been achieved. Recently, nanotechnology has presented an excellent method to accelerate acute and chronic wound healing by appropriate movement through the various healing stages. The ability of nanoparticles (NPs) to act as therapeutic and carrier systems they consider an efficient treatment strategy for wound healing. Their small size and high surface area to volume ratio enhance the probability of bio-interaction and penetration at the wound area aiding cell-cell interactions, the proliferation of cells, cell signaling, and vascularization.

P-38/ICC-04-23

## Convergent Synthesis, Kinetics Insight and Computational Attributions of Thiazole-(5-aryl)oxadiazole Hybrids Encompassed with Propanamides as Alkaline Phosphatase Inhibitors

**Zareen Fatima**

*Department of Chemistry, Government College University Lahore*

**Abstract:**

Considering the varied pharmacological prominence of thiazole and oxadiazole heterocyclic moieties, a unique series of bi-heterocyclic hybrids, **8a-h**, was synthesized in a convergent manner. The structures of newly synthesized compounds were characterized by $^{1}$H-NMR, $^{13}$C-NMR, and IR spectral studies. The structure-activity relationship of these compounds

was predicted by examining their inhibitory effects against alkaline phosphatase, whereby all these molecules exhibited superb inhibitory potentials relative to the standard used. The Kinetics mechanism was determined by Lineweaver-Burk plots which revealed that, **8g**, inhibited the studied enzyme non-competitively by forming an enzyme-inhibitor complex. The inhibition constants $K_i$ calculated from Dixon plots for this compound was 0.42 µM

P-39/ICC-04-23

## Synthesis, characterization and biological screening of S-substituted derivatives of 5{1-[(4-methylphenyl)sulfonyl]-4-piperidinyl}-1,3,4-oxadiazole-2-thiol

**Zeeshan Munir, Dr Aziz Ur Rehman**

*Department of Chemistry, Government College University, Lahore*

**Abstract:**

To synthesize biologically active compounds bearing three highly active moieties in one core i.e. 1,3,4-oxadiazole,sulphonyl group and piperidine ring. In the following research series of different S-substituted derivatives of 5{1-[(4-methylphenyl)sulfonyl]-4-piperidinyl}-1,3,4-oxadiazole-2-thiol were synthesize in five steps. In the first step, Ethyl-1-[(4-methylphenyl)sulfonyl]-4-piperidinecarboxylate (1) was synthsized from 4-methylbenzenesulfonylchloride (a) and Ethyl-4-piperidinecarboxylate (b). In the second and third step, compound 1 was converted into Ethyl-1-[(4-methylphenyl)sulfonyl]-4-piperidinecarbohydrazides (2) and 5-{1-[(4-methylphenyl)sulfonyl]-4-piperidinyl}-1,3,4-oxadiazole-2-thiol(3) respectively. In fourth step, variety of different arylamine (4a-i) were treated with 2-bromopropionylbromide to produce series of propanamide (5a-i) which were acted as electrophile in undertaken procedure. In the final step, 5{1-[(4-methylphenyl(sulfonyl]-4-piperidinyl}-1,3,4-oxadiazole-2-thiol (3) and propanamide (5a-i) were reacted to obtain 9 different S-substituted derivatives of 5{1-[(4-methylphenyl(sulfonyl]-4-piperidinyl}-1,3,4-oxadiazole-2-thiol (5a-i) respectively. Purity and structure of all synthesize compounds were justified by the help of IR , $^{1}$H-NMR , $^{13}$C-NMR and EIMS spectral data. The series was also tested for different biological activities.

P-40/ICC-04-23

## Eco friendly Synthesis of silver nanoparticles for antimicrobial applications

**Ayesha Khalid**

*Department of Biology, Lahore Garrison University, Lahore*

**Abstract:**

The aim of this study was to make antimicrobial silver nanoparticles and related materials for the eradication of microbes hence preventing the nosocomial infection. Multi drug resistance is the promising challenge of this era. For this purpose, two plant sources were used for green synthesis of silver nanoparticles. No chemicals or high energy optimization conditions were required. Silver nanoparticles were prepared by using sunlight and room temperature. The clinical bacterial isolates, collected from the medical equipment were used to study the antimicrobial potential of AgNPs. AgNPs possessed significant antimicrobial inhibition. Silver nanoparticles were immobilized over cotton thread, cotton fabric and diaphragm of stethoscope and then the bacterial load was again estimated.

P-41/ICC-04-23

## Smart Bioadhesives for Wound Healing and Closure

**Arqam Tahir, Abdullah Zahid, Zainab Noor, Samia Baig and Hammad Arshad**

*Department of Biology, Lahore Garrison University*

**Abstract:**

The increasing demand for rapid wound healing has spiked the development of smart and multifunctional bioadhesives having properties such as strong bioadhesion, real-time sensing, antibacterial activity, and wireless-on-demand drug release capabilities, etc. Accelerated wound healing can be achieved through direct release of antimicrobial and growth factors, and delivery of curative cells. Recently, the integration of treatment modules and biosensing with wireless units in a closed-loop system has produced smart bioadhesives which allow real-time sensing and monitoring of the physiological conditions (e.g., pH, and temperature) as well as stage-specific wound healing by triggering on-demand-drug delivery and treatment to avoid any probable infections or prolonged inflammation. Despite of some

major advances in this field, challenges in the design and fabrication of integrated systems, especially for chronic wounds, still exist which present significant opportunities for the future development of next-generation smart materials and systems.

P-42/ICC-04-23

## Nanoparticle-based therapeutic approaches for wound healing

**Aleena Zainab, Aleesha Naheed, and Hammad Arshad**

*Department of Biology, Lahore Garrison University, Lahore*

**Abstract:**

Wound healing is a complicated anatomical procedure and is challenging. As reported, many coexisting diseases (diabetes, vascular diseases, etc.) significantly impact wound healing. Factors like repetitive injury, age, or hypertrophic scarring also affect wound healing. During the last years, the improvement of wound dressing biomaterials has registered a new standard level and superior knowledge based on chronic wound pathogenesis has been achieved. Recently, nanotechnology has presented an excellent method to accelerate acute and chronic wound healing by appropriate movement through the various healing stages. The ability of nanoparticles (NPs) to act as therapeutic and carrier systems they consider an efficient treatment strategy for wound healing. Their small size and high surface area to volume ratio enhance the probability of bio-interaction and penetration at the wound area aiding cell-cell interactions, the proliferation of cells, cell signaling, and vascularization.

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P-43/ICC-04-23

# Targeting the main protease (Mpro) of SARS-CoV-2 for discovering anti COVID-19 therapeutics

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**Abstract:**

The COVID-19 pandemic has claimed 6.87 million lives worldwide within a short time span. Due to unavailability of specific antiviral drugs, critically sick patients of COVID-19 are at the risk of developing multiorgan failure syndrome and higher mortality rate. Despite the discovery of vaccines against the causative agent SARS-CoV-2, the chances of breakthrough infections are on rise due to emergence of several new viral strains. Therefore, an urgent discovery and development of effective antiviral drug for the treatment of COVID-19 is highly desired. Towards this objective, several viral enzymatic proteins including the main protease (Mpro), papain-like protease (PL-pro), and RNA dependent RNA polymerase (RDRP) offers unique opportunity for discovering leads that could be developed into specific antivirals. To address this challenge, a recent development in medicinal chemistry is the novel strategy of Fragment-Based-Drug-Discovery (FBDD). Screening small fragment libraries of diverse scaffolds against the viral proteins as drug targets using biophysical techniques is becoming a hot area of medicinal chemistry research due to its faster rate of hit identification and wider range of chemical space coverage. Certain heterocyclic rings including pyrrole, thiazolidinone and quinolone have been proved privileged structural moieties and appear frequently in the structures of viral protease inhibitors. In this poster, we will disclose our finding on the synthesis and biological evaluation of selected pyrroles and thiazolidinones against SARS-COV-2 Mpro protease.

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# Synthesis of a bifunctional catalyst (Cobalt Iron Borate (CoFeB)) for hydrogen generation from alkaline sodium borohydride and catalyzing the reduction of 4-Nitrophenol

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**Abstract:**

Burning fossil fuels to meet energy demands, contributes to global warming and climate change, so alternative renewable energy sources are needed. Hydrogen is a promising energy carrier, and Sodium Borohydride ($NaBH_4$) is a promising hydrogen storage material. However, developing an efficient catalyst for NaBH4 hydrolysis to generate hydrogen is challenging. We propose investigating the efficiency of cobalt-based catalysts for NaBH4 hydrolysis. Cobalt Iron borate (CoFeB) is a bifunctional catalyst that generates hydrogen from NaBH4 and reduces 4-nitrophenol. We used X-ray diffraction (XRD) and scanning electron microscopes (SEM to examine the structural and morphological features of the catalyst. The highest hydrolysis rate observed for Co- Fe-borate is 1357.62 ml.min-1 0.5g-1 with 1 wt% NaBH4, 1M NaOH solution at 25°C with an activation energy of 11.68 kJ mol-1. Furthermore, the optimized material demonstrates excellent catalytic capability with an apparent rate constant (kapp) of 32.62 ×10-3 s-1. These findings indicate that CoFeB possesses potential applications in both sodium borohydride hydrolysis and reduction of 4-nitrophenol, comparable to precious metal-based catalysts.

P-45/ICC-04-23

## Synthesis and Characterization of Spiroisatin-based Novel Compounds of Medicinal Interest

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**Abstract:**

Based on the gilt-edged biological activities of spiro[indoline-3,2'-[1,3]dioxolan]-2-one (I-1) and other isatin derivatives, the project was designed to make spiroisatin-based compounds by forming a spiro-ketal at position 3 of isatin. First step involves the synthesis of 2-(2-oxospiro[indoline-3,2'-[1,3]dioxolan]-l-yl)acetohydrazide (I-3) in excellent yield. Using this novel hydrazide of spiroisatin three different series were synthesized. In first series different aromatic aldehydes were condensed with (I-3) to form their respective hydrazones (I-5at). To synthesize the second and third series, electrophilic components were synthesized. These N-alkylated isatin (I-6a-o) and isatin bearing N-phenylacetamides (I-9a-u) were then condensed with (I-3) to synthesize the targeted hydrazones (I-7a-o) and (I-10a-u). These synthesized compounds were characterized and confirmed using (FT-IR, 1H NMR, 13C NMR, LC-MS spectroscopy). Drugs like properties were studied using SwissADME, and Molinspiration. DFT calculations were done using Gaussians View 9.0. After complete characterization these synthesized compounds will further be screened for biological activities and structure activity relationship (SAR) will be noted

P-46/ICC-04-23

## Targeting NS2BNS3 protease of Dengue Virus for the discovery of early phase antiviral drugs

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**Abstract:**

Intermittent Dengue virus (DENV) infections has become very common in Pakistan since 2011. About half of the world population, living in the tropical and sub-tropical regions, is

directly under the threat of DENV infection, whereas the remaining is under indirect threat due to international travel and global warming. According to WHO an estimated 100-400 million infections occur each year, over 80% are generally mild and asymptomatic. There is still no specific antiviral treatment available against these infections. Therefore, discovery and development of a specific anti-dengue therapeutic is highly demanding area of research. Dengue virus is composed of RNA-based genome, which is translated in the host cell into a single polyprotein. The polyprotein must be co- and post-translationally processed into mature viral proteins to produce infective virions. A viral protein, namely NS2B/NS3 protease is responsible for this task and thus provide an efficient target for the early phase discovery of antiviral drug. Thus, using a recombinantly expressed viral protease, we embarked on testing newly synthesized heterocyclic compounds containing pyrazole scaffold. Owing to its high biological importance, we have constructed structurally diverse pyrazoles and tested their inhibitory potential against DENV biochemical assay. In this poster, we will disclose the results of biochemical screening and computational delineation of protease-inhibitor interaction map. These findings will play an important role in our effort toward the discovery and development of antivirals against DENV infections.

P-47/ICC-04-23

## A Convergent Synthesis of the Pyrazolone based Hetarylidenes as New Antioxidant Agents

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**Abstract:**

The accumulation of free radicals can damage the cells, which may instigate dangerous diseases in human beings. Therefore, contribution of antioxidants in scavenging or minimizing the impacts of such free radicals is of great significance. Different research studies have claimed that heterocyclic nuclei are the core elements in the structural frameworks of many potent antioxidant pharmacophores. In this context, the present study was thus designed in which an ultrasound mediated facile synthetic approach was adopted to

prepare some hetarylidenes **3**(**a-h**) engineered with the pyrazolone motif followed by the preliminary in vitro evaluation of radical scavenging potentials of these synthesized scaffolds. The sonication process assisted this condensation reaction very well and improved the results both in terms of product yields (up to 92%) as well as in reaction times (45-60 min) in comparison with our prior findings. Afterwards, the synthesized derivatives were screened out for their antioxidant potentials against DPPH free radical. Overall, this series displayed moderate to good free radical scavenging activity. The observed structure-antioxidant activity relationship could be considered for further in-depth investigations.

P-48/ICC-04-23

## Mixed Chelating Agents for the Removal of Heavy Metals from Flooded Soil

**Khansa Zafar, Muhammad Dilshad, Iqra Zubair Awan**

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**Abstract:**

Accumulations of heavy metals such as As, Pb, Hg and Cr in the soil and plants have harmful impacts on the physiological activities of plants such as photosynthesis, gaseous exchange, and nutrient absorption which reduce the plant growth and result in dry matter accumulation. Heavy metals also have intense effects on human's health and other living organisms through food chain and may causes many diseases for instance, gastrointestinal and kidney dysfunction, nervous system disorders, skin lesions, vascular damage, immune system dysfunction, birth defects, and cancer are examples of the complications of heavy metals toxic effects. To remove heavy metals from the soil organic acid are more efficient and environment friendly because there is no production of harmful oxides like $SO_2$, $NO_2$ and $Cl_2$. In this context, we have experimented the effectiveness of oxalic and citric acid for the removal of As, Pb and Cr in the recent flood effected soil samples at a range of concentration, pH and temperature. The samples were then analyzed by Atomic Absorption Spectroscopy (AAS) and Inductively Coupled Plasma (ICP) techniques.

P-49/ICC-04-23

## A Novel Method of Metal Recovery from Rotten Fruit Extracts

**Fakiha Azeem, Muhammad Dilshad, Iqra Zubair Awan**

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**Abstract:**

Fruits have essential nutrients that are necessary for us but unfortunately, nearly half of the fruits due to improper handling are wasted each year worldwide. These rotten fruits are rich in important metals and these metals can be leached out by using organic acid and can be used for different purpose. Metals form coordinate covalent bond with the chelating agent. Organic acids such as oxalic acid is an efficient and environmental friendly bidentate agent then inorganic acids because there is no production of harmful oxides like $SO_2$, $NO_2$ and $Cl_2$. In this work, we have developed a procedure to extract Potassium (K) & Iron (Fe) from rotten Guava, Magnesium (Mg) from Apple, and Potassium (K) & Calcium (Ca) from Banana. Three parameters, pH (2-4), concentration of oxalic acid (0.1M - 1M) and temperature (45℃ - 85℃) were studied. After leaching sample were analyzed by Atomic Absorption Spectroscopy (AAS) and Inductively Coupled Plasma (ICP). The results indicated significant leaching of metals from the respective fruits.

P-50/ICC-04-23

## Use of *Epipremnum aureum* for the removal of chromium from water in association with chromium-resistant microbes

**Rizwana Fatima, Zaiba Amanat, Muhammad Usman, and Sumaira Mazhar**

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**Abstract:**

More than 800 tannery industries in Pakistan discharge untreated industrial effluents leading to contamination of nearby soil, aquatic life, groundwater quality, and humans by noxious heavy metals and other contaminants. The current study was designed to evaluate the potential of *Epipremnum aureum* in chromium removal from water in association with

chromium-resistant microbes. Wastewater samples were collected from different tannery industries in Pakistan to isolate chromium-resistant microbes. *Epipremnum aureum* plants were collected from DHA Phase 6 nursery in Lahore, Pakistan. Bacteria isolated from collected wastewater samples showing the highest resistance against chromium were characterized morphologically and biochemically using standard microbiological techniques. Non-inoculated and inoculated *Epipremnum aureum* plants with selected bacterial isolates were grown in nutrient broth media supplemented with different concentrations of chromium. Following 5 to 10 days, the chromium reduction potential of both inoculated and non-inoculated plants was recorded. *Epipremnum aureum* plants have the potential to remove chromium from water and it increased in the presence of chromium-resistant microbes.

P-51/ICC-04-23

**Phytoremediation of lead contaminated soil by using sorghum plant in association with the indigenous microbes**

**Iqra Tabbasa and Sumaira Mazhar**

*Department of Biology, Lahore Garrison University. Lahore, Pakistan*

**Abstract**

Heavy metals are being discharged in large quantities in land and water bodies, causing long-term damage to living organisms. Phytoremediation is an effective way to address this problem. The goal of this study was to identify that how lead resistant microorganisms affected sorghum plant growth in the presence of lead and in the absence of lead. Isolation and characterization of lead resistant microbes were isolated from sorghum plant to investigate growth and concentration of lead with in the sorghum plant. Isolated species were inoculated with lead containing media in different concentrations i.e. 300, 400, 500 and 600µg/ml. Highly lead resistant bacterial isolates were selected and inoculated with sorghum seeds under typical environmental conditions in small pots with and without lead contamination (300mg/Kg). In presence of lead resistant bacteria efficient growth were observed with less concentration of lead in sorghum plants. Promising results were observed

in presence of GS3 and IS2 isolates. Current study showed that lead tolerant bacterial isolates were very helpful to degrade lead when grown with sorghum seeds and it also enhances growth of sorghum plant.

P-52/ICC-04-23

## Synthesis of Chalcones and their Antimicrobial Efficacy against Pathogens

**Tariq Nawaz, Ayesha Waheed Qureshi, Affifa Tajammal**

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**Abstract:**

Novel antimicrobial agents are required to treat the threat of drug-resistant microbes. The emergence of fighting of multidrug resistant microbes against the antimicrobial drugs has fueled research attention in the way of designing new scaffolds as well as strategies to counter the drug resistance. Chalcones with their broad-spectrum biological activities are proved to be better candidate in this respect. Four chalcones were synthesized by Claisen Schmidt condensation and structures were confirmed by IR, $^{1}$H NMR and $^{13}$C NMR. The synthesized compounds were screened for antibacterial and antibiofilm activities. Compounds 79 (at conc. 50 µg) showed the highest antibacterial activity against pathogens (E. coli, K. pneumoniae and S. aureus) as compared to the reference drug Ciprofloxacin (30 µg/ml) while this compound showed 27 mm ZOI against P. aeuroginosa which is near to reference drug Ciprofloxacin. Compound 82 (at conc. 50 µg) showed the highest antibacterial activity against pathogens (E. coli, P. aeuroginosa, K. pneumoniae and S. aureus) compared to the reference drug Ciprofloxacin (30 µg/ml). But this compound showed 19 mm zone against K. pneumoniae which is near to reference drug Ciprofloxacin. The compounds 79 (at conc. 30 µg), 80 (at conc. 30 µg) and 82 (at conc. 50 µg) has showed highest significant results ($P > 0.05$) of biofilm inhibition efficacy against for all pathogens (E. coli, P. aeuroginosa, K. pneumoniae and S. aureus) compared to the reference drug Ciprofloxacin (30 µg/ml).

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# Phytochemical Screening and Antimicrobial Studies of *Carica papaya* fruit and peel extract and their role in synthesis of Silver Nanoparticles

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**Abstract:**

Ethanolic extracts of Fruit (pulp) and the peel of the *Carica papaya* were prepared and subjected to qualitative and quantitative phytochemical screening. These extracts were used to prepare silver nanoparticles and evaluated for their antibacterial potential against gram +ve and gram-ve bacteria. For this purpose, 4 different extracts of each of the two samples were prepared by grinding, boiling under high pressure, soaking and refluxing using water and ethanol as solvent. All the extracts were found to have Carbohydrates, Flavonoids, Phytosterols, Cardiac glycosides and protein whereas quantitative analysis of the flavonoid by aluminium colorimetric method revealed that PR (0.1323 mg/g QE) contained highest flavonoid concentrations whereas the lowest concentration was found in PER (0.0017 mg/g QE). Flavonoid content was not detected in other samples. To evaluate the catalytic potential of these extracts in reduction of silver ions and stabilization of its nanoparticles, extracts were treated with silver nitrate solution in basic media at room temperature and 50°C. AgNPs were characterized by UV/VIS spectroscopy. All extracts and AgNPs were evaluated for their antimicrobial potential against the *E. coli* and *S. aureus* by well diffusion method and zones of inhibition were measured. The maximum antibacterial activity was observed by FR showing maximum zone of inhibition (28.0 mm) against *E. coli* and (22.0 mm) *S. aureus.*

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# Study on adulteration and composition of milk sold at Lahore

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**Abstract:**

Milk adulteration is one of the major global concerns as milk is consumed as a healthy dairy product everywhere in the world. Adulteration of milk is an increasingly common fraudulent practice. This research was conducted to investigate various adulterations and their effects on the chemical properties of market milk supplied in Lahore. 20 milk samples from each milk producer (MP), milk collector (MC), milk vendor (MV), and dairy shop (DS) were collected and tested for various adulterants (water, urea, starch, detergents, cane sugar, formalin, and skimmed milk powder). The majority of milk samples contained only water out of these adulterants.80% of milk samples of MP, 75% of milk samples of MC, 95% of milk samples of MV, and 100% of milk samples of DS showed freezing points that were closer to 0°C than control milk's (-0.55°C). The chemical properties of milk showed a mean substantial influence from extraneous water. Except for MC milk, the moisture level of milk from various intermediaries was much higher than that of control milk. Milk from MP was noticeably higher in fat content than milk from MC, MV, and DS and the fat content of milk sold by various intermediaries was not comparable to control milk samples. When compared to MP, MV, and DS milk, the average protein concentration of MC milk was found to be noticeably higher, and none of these milk samples was similar to control milk in terms of protein content. Despite the fact that the average lactose content of milk from MP, MC, and DS was found to be lower than that of control milk, it did not demonstrate any appreciable effects of extraneous water, whereas the lactose content of milk was affected. The ash level of MC, MV, and DS milk was noticeably altered, the ash content of MP milk looked to be very similar to that of control milk. Extraneous water was ultimately determined to be the only adulterant in market milk at Lahore that significantly changed the chemical composition of milk.