22nd International and 34th National Chemistry Conference

October 30-November 01, 2024

Chemistry for Sustainable Life

DEPARTMENT OF CHEMISTRY
UNIVERSITY OF MALAKAND
KHYBER PAKHTUNKHWA, PAKISTAN

ABOUT THE CONFERENCE

Welcome to Chemcon 2024

Department of Chemistry is thrilled to extend a warm invitation to all participants for the upcoming "22nd International & 34th National Chemistry Conference", scheduled to take place from October 30th to November 1st, 2024, in University of Malakand, Khyber Pakhtunkhwa with the theme "Chemistry for Sustainable Life" , this conference promises to be an enriching experience for all involved.

Our meticulously designed scientific tracks are geared towards offering attendees a profound learning experience. Chemcon 2024 aims to bring together distinguished scientists, emerging researchers, educators, healthcare professionals, business delegates, and exceptional student communities from around the globe for a robust exchange of ideas. It's a platform where researchers and authors can showcase their work amidst a stimulating atmosphere of dialogue and collaboration.

The conference will feature a comprehensive program including plenary sessions, Keynote addresses, Invited lectures, and Oral/Poster presentations. We are confident that this gathering will be both intellectually rewarding and foster valuable collaborations among participants.

Chemcon-2024 will provide a forum to showcase recent advancements and front-line chemistry and material sciences research. It will be a significant platform for researchers, academicians, and students to engage in knowledge and technology sharing. This conference will also encourage participants to reciprocate experiences and debate on the current research challenges. Besides, it will provide an opportunity to promote future collaboration and knowledge transfers between participants. It will include keynote lectures, invited talks, and oral presentations on different topics of current interest. This event will also identify prolific opportunities for future research in chemistry and materials.

The influential topics will cover a broad spectrum including all aspects of chemistry and allied sciences.

- Analytical Chemistry
- Applied Chemistry
- Biochemistry
- Computational Chemistry
- Environmental Chemistry
- Food Chemistry
- Green Chemistry
- Inorganic Chemistry
- Organic Chemistry
- Physical Chemistry
- Renewable Energy

Patron in Chief

Prof. Dr. Atta-ur-Rahman (FRS, N.I, H.I, S.I, T.I, UNESCO Science Laureate)

Professor Emeritus, H.E.J. Research Institute of Chemistry University of Karachi

Patron

Prof. Dr. Rashid Ahmad

Vice Chancellor, University of Malakand

Chief Organizer

Prof. Dr. Sultan Alam

Chairman, Department of Chemistry, University of Malakand

Deputy Chief Organizer

Dr. Muhammad Sadiq

Associate Professor, Department of Chemistry, University of Malakand

Conference Focal Person

Dr. Mumtaz Ali

Associate Professor, Department of Chemistry, University of Malakand

Organizing Secretary

Dr. Mian Muhammad

Associate Professor, Department of Chemistry, University of Malakand

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ADVISORY COMMITTEE

1. **Prof. Dr. Atta-ur-Rahman** (FRS, N.I, H.I, S.I, T.I, UNESCO Science Laureate)
   Professor Emeritus, H.E.J. Research Institute of Chemistry University of Karachi
2. **Prof. Dr. Rashid Ahmad**
   Vice Chancellor, University of Malakand
3. **Prof. Dr. Muhammad Rasul Jan** (Pride of Performance, S.I)
   Professor Emeritus, ICS, University of Peshawar
4. **Prof. Dr. M. Iqbal Choudhary** (H.I, S.I, T.I)
   Meritorious Professor, H.E.J. Research Institute of Chemistry
   University of Karachi
5. **Prof. Dr. Iftikhar Ahmad** (T.I)
   Meritorious Professor/ Director, Center for Computational Materials Science, University of Malakand
6. **Prof. Dr. Rahmat Ali**
   Vice Chancellor, Kotli University
7. **Prof. Dr. Gul Zaman**
   Professor/Dean of Sciences, University of Malakand
8. **Prof. Dr. Ch. Jamil Anwar**
   Distinguished University Professor, School of Science, Department of Chemistry, UMT, Lahore
9. **Prof. Dr. Jasmin Shah**
   Meritorious Professor, ICS, University of Peshawar
10. **Prof. Dr. Raza Shah** (T.I)
    Professor, International Center for Chemical and Biological Sciences, H.E.J. Research Institute of Chemistry University of Karachi
11. **Prof. Dr. Safeer Ahmed**

Quaid-i-Azam University, Islamabad

SCIENTIFIC COMMITTEE

1. Prof. Ahmet Tutar
   Department of Chemistry, Faculty of Science, Sakarya University, Turkiye
2. Prof. Bagher Eftekhari-Sis,
   Professor, Department of Chemistry, University of Maragheh, Iran
3. Dr. Maryam Zirak
   Associate Professor, Organic Chemistry, Payame Noor University, Iran
4. Prof. Dr. Imtiaz Ahmad
   Professor, ICS, University of Peshawar
5. Prof. Dr. Jan Nisar
   Professor, NCE in Physical Chemistry, University of Peshawar
6. Prof. Dr. Irshad Hussain
   Professor, Department of Chemistry & Chemical Engineering, SBA School of Science & Engineering, Lahore University of Management Science
7. Prof. Dr. Ezzat Khan
   Professor, Department of Chemistry, University of Bahrain
8. Prof. Dr. Sultan Alam
   Chairman, Department of Chemistry, University of Malakand
9. Prof. Dr. Zia Ur Rahman
   Quaid-i-Azam University, Islamabad

PLENARY SPEAKERS

Prof. Dr. Atta Ur Rahman (FRS, N.I, H.I, S.I, T.I, UNESCO Science Laureate)

Patron Chemical Society of Pakistan

Prof. Dr. Muhammad Khwaja Nazeeruddin

Institut des Sciences et Ingenierie Chimiques. École Polytechnique Fédérale de Lausanne, Sion, Switzerland

Prof. Dr. Raza Shah

HEJ, University of Karachi, President Chemical Society of Pakistan

Prof. Dr. Mohammad Rasul Jan

Professor Emeritus, University of Peshawar

Prof Dr. Iqbal Choudhary

National Distinguished Professor, University of Karachi

Prof Dr. Irshad Hussain

Lahore University of Management Sciences Lahore

Prof. Dr. Islamullah Khan

Vice Chancellor, University of Mianwali, Pakistan

INVITED/KEYNOTE SPEAKERS

Prof. Asharf Ghaneem,

Molecular & Biochemical Therapeutics, Faculty of SciTech, University of Canberra, Australia

Prof. Ali Alkan, Karadeniz

Technical University, Institute of Marine Science and Technology, Trabzon, Türkiye

Prof. Ahmet Tutar

Department of Chemistry, Faculty of Science, Sakarya University, Sakarya, Türkiye

Bagher Eftekhari-Sis

University of Maragheh, Iran

Prof. Iftikhar Ahmad

Meritorious Professor, University of Malakand

Prof. Dr. Hassan Sher

Vice Chancellor University of Swat

Dr. Najeeb Ullah

CEO Edison Innovation Venture and Services (A Venture Accelerator), St John Innovation Center Cambridge and Serena Business Complex Islamabad, Pakistan

Prof. Safer Ahmad

Department of Chemistry Quaid e Azam University Islamabad, Pakistan

Prof. Haq Nawaz Bhati

University of Agriculture Faisalabad, Pakistan

Prof. Jameel Anwar

Distinguished University Professor, School of Science, Department of Chemistry, UMT, Lahore

Prof. Dr. Humaira Yasmeen Gondal

Institute of Chemistry, University of Sargodha

Dr. Shahzad Ali Shahid Chatha

Professor, Government College University Faisalabad

Prof. Dr. Imran Din

School of Chemistry, University of the Punjab

Prof. Dr. Adnan Mujahid

School of Chemistry, University of the Punjab

Prof. Dr. Muhammad Zaman Ashraf

Department of Chemistry, Rawalpendi Women University Islamabad

Prof. Dr. Adeel Afzal

School of Chemistry, University of the Punjab

Prof. Dr. Muhammad Arshad

Professor of Organic Chemistry, Institute of Chemistry, The Islamia University of Bahawalpur

ORGANIZING COMMITTEES

1. Media/ Information Committee

1.	Dr. Mian Muhammad	Convener
2.	Mr. Masaud Hassan	Member
3.	Dr. Muhammad Zahid Khan (Media Cell)	Member
4.	Mr. Jamil Anwar Abbasi (Media Cell)	Member
5.	Mairaj ul Hamid Nasri, PRO	Secretary

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1.	Dr. Hazrat Ali	Convener
2.	Dr. Faiz Ali	Member
3.	Dr. Muhammad Said	Member
4.	Dr. Abdul Latif	Member
5.	Dr. Hira Zaman	Member

3. Finance Committee

1.	Dr. Abdul Latif	Convener
2.	Dr. Muhammad Said	Member
3.	Dr. Faiz Ali	Member
4.	Director Finance, UOM	Member
5.	Chief Auditor UOM	Member

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1.	Prof. Dr. Rashid Ahmad	Convener
2.	Prof. Dr. Attaur Rahman	Member
3.	Prof. Dr. Iftikhar Ahmad	Member
4.	Prof. Dr. Mir Azam Khan	Member
5.	Prof. Dr. Sultan Alam	Member
6.	Prof. Dr. Gul Zaman	Member
7.	Prof. Dr. Waqar Ahmad	Member

5. Registration/Reception Committee

1.	Dr. Faiz Ali	Convener
2.	Dr. Abdul Latif	Member

3. Dr. Muhammad Said	Member
4. Dr. Hazrat Ali	Member
5. Dr. Hafiz A. W. Kamran	Member
6. Dr. Hira Zaman	Member

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3. Dr. Muhammad Naveed Umar	Member
4. Dr. Maria Sadia	Member
5. Dr. Haseena	Member
6. The Provost/Deputy Provost, UOM	Member

7. Food and Refreshment Committee

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2. Dr. Hanif Khan	Member
3. Prof. Dr. Mir Azam Khan	Member
4. Dr. Manzoor Ahmad	Member
5. Dr. Muhammad Sadiq	Member
6. Dr. Maria Sadia	Member

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1. Dr. Muhammad Naveed Umar	Convener
2. Dr. Muhammad Sadiq	Member
3. Dr. Muhammad Said	Member
4. Dr. Faiz Ali	Member
5. Director, ORIC, UOM	Member

9. Transportation Committee

1. Prof. Dr. Sultan Alam	Convener
2. Dr. Mian Muhammad	Member
3. Inch. Transport	Member
4. Dr. Abdul Waheed Kamran	Member
5. Dr. Faiz Ali	Member
6. Visiting Teaching Faculty	Member

7.	MPhil/PhD Scholars	Member

10. Logistics Committee

1.	Dr. Muhammad Sadiq	Convener
2.	Dr. Manzoor Ahmad	Member
3.	Dr. Sultan Alam	Member
4.	Dr. Mumtaz Ali	Member
5.	Dr. Abdul Waheed Kamran	Member

11. Security Committee

1.	Director Administration UOM	Convener
2.	Provost UOM	Member
3.	Dr. Muhammad Naveed Umar	Member
4.	In-charge University Police	Member
5.	In-charge Elite Police Force	Member
6.	Chief Proctor UOM	Member
7.	Mr. Dost Muhammad	Member

Conference Program (Chemcon-2024)

DAY-1; Wednesday, October 30, 2024

TIME	ACTIVITY		
09:00 - 10:00	**REGISTRATION (Department of Chemistry, UOM)**		
10:00 - 11:30	Inauguration of the Conference (Convocation Hall)		
	Recitation of The Holy Quran/National Anthem		
	Address by the Chief Organizer		
	Address by the President CSP		
	Address by the Patron-in-Chief		
	Address by the Chief Guest		
	Shields distribution and CSP Awards		
11:30 - 12:00	**REFRESHMENT BREAK**		
12:00 -12:30	Plenary Lecture-01**(Virtual)** **Prof. Dr. Atta Ur Rahman** Patron Chemical Society of Pakistan (Venue: Convocation Hall, UOM)		
12:30-13:00	Plenary Lecture-02 (Virtual) **Prof. Dr. Muhammad Khwaja Nazeeruddin** École Polytechnique Fédérale de Lausanne, Sion, Switzerland (Venue: Convocation Hall, UOM)		
13:00 - 13:30	Plenary Lecture-03 **Prof Dr. Iqbal Choudhary** National Distinguished Professor, University of Karachi (Venue: Convocation Hall, UOM)		
13:30 - 14:00	Plenary Lecture-04 **Prof. Dr. Raza Shah** HEJ University of Karachi, President Chemical Society of Pakistan (Venue: Convocation Hall, UOM)		
14.00 - 15:00	**LUNCH**		
15:00 - 17:00	**Technical Session-1**		
15:00 - 15:30	**Invited Speech/Keynote Lecture-1**		
	(1a) Prof. Dr. Iftikhar Ahmad Meritorious Professor, University of Malakand	**(1b) Prof. Dr. Haq Nawaz Bhati** University of Agriculture Faisalabad, Pakistan	**(1c) Prof. Dr. Hassan Sher** Vice Chancellor University of Swat
15:30 - 17:00	Technical Session-1a – Physical, Inorganic & Analytical Chemistry		
15:30 - 17:00	Technical Session-1b – Organic & Biochemistry		
15:30 - 17:00	Technical Session-1c – Applied, Theoretical & Environmental Chemistry		
17:00-18:30	**REFRESHMENT BREAK**		
18:30 -19:00	**Technical Session-1 (Continued)**		
19:00-20:00	**General body meeting of The Chemical Society of Pakistan**		
20:00 - 21:00	**DINNER**		

Conference Program (Chemcon-2024)

DAY-2; Thursday, October 31, 2024

09:00 - 09:40	Plenary Lecture-05 **Prof. Dr. Mohammad Rasul Jan** Professor Emeritus, University of Peshawar (Venue: Convocation Hall, UOM)		
09:40 - 10:20	Plenary Lecture-06 **Dr. Najeeb Ullah** CEO Edison Innovation Venture and Services (A Venture Accelerator), St John Innovation Centre Cambridge and Serena Business Complex Islamabad, Pakistan (Venue: Convocation Hall, UOM)		
10:20 - 11:00	**REFRESHMENT BREAK**		
11:00 - 13:00	**Technical Session-2**		
11:00 - 11:30	**Invited Speech/Keynote Lecture**		
	(2a) Prof. Dr. Tajnees Pirzada Shah Abdul Latif University, Khairpur Sindh, Pakistan	**(2b) Prof. Dr. Imran Din** School of Chemistry University of the Punjab	**(2c) Prof. Safer Ahmad** Department of Chemistry Quaid e Azam University Islamabad, Pakistan
11:30 - 13:00	Technical Session-1a – Physical, Inorganic & Analytical Chemistry		
11:30 - 13:00	Technical Session-1b – Organic & Biochemistry		
11:30 - 13:00	Technical Session-1c – Applied, Theoretical & Environmental Chemistry		
13:00 - 14:00	**LUNCH BREAK**		
14:00 - 16:00	**Technical Session-3**		
14:00 - 14:30	**Invited Speech/Keynote Lecture**		
	(3a) Prof. Dr. Adnan Mujahid School of Chemistry University of the Punjab	**(3b) Prof. Dr. Adeel Afzal** School of Chemistry University of the Punjab	**(3c) Prof. Dr. Muhammad Arshad** Institute of Chemistry the Islamia University of Bahawalpur
14:30 - 16:00	Technical Session-1a – Physical, Inorganic & Analytical Chemistry		
14:30 - 16:00	Technical Session-1b – Organic & Biochemistry		
14:30 - 16:00	Technical Session-1c – Applied, Theoretical & Environmental Chemistry		
16:00-16:30	**REFRESHMENT BREAK + POSTER EXHIBITION**		
16:30 - 18:00	**Technical Session-3 (Continued)**		
19:00 – 19:30	Plenary Lecture-07 (Virtual) **Prof. Bagher Eftekhari-Sis** University of Maragheh, Iran (Venue: Convocation Hall, UOM)		
19:30 – 20:00	Plenary Lecture-08 (Virtual) **Prof. Ahmet Tutar** Department of Chemistry, Faculty of Science, Sakarya University, Türkiye (Venue: Convocation Hall, UOM)		
20:00 - 21:00	**DINNER**		

Conference Program (Chemcon-2024)

DAY-3; Friday, November 01, 2024

<table>
<tr><td>9:00 – 12:00</td><td colspan="3">Technical Session-4</td></tr>
<tr><td rowspan="2">9:00 - 9:30</td><td colspan="3">Invited Speech/Keynote Lecture</td></tr>
<tr><td>(4a) Prof. Dr. Muhammad Zaman Ashraf
Rawalpindi Women University Islamabad</td><td>(4b) Prof. Dr. Shahzad Ali Shahid Chatha
Government College University Faisalabad</td><td>(4c) Prof. Dr. Humaira Yasmeen Gondal
Institute of chemistry, University of Sargodha</td></tr>
<tr><td>9:30 - 11:30</td><td colspan="3">Technical Session-1a – Physical, Inorganic & Analytical Chemistry</td></tr>
<tr><td>9:30 - 11:30</td><td colspan="3">Technical Session-1b – Organic & Biochemistry</td></tr>
<tr><td>9:30 - 11:30</td><td colspan="3">Technical Session-1c – Applied, Theoretical & Environmental Chemistry</td></tr>
<tr><td>11:30 - 12:00</td><td colspan="3">CLOSING SESSION & Farewell to the Guests</td></tr>
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Technical Sessions

Technical Session-1a - Physical, Inorganic & Analytical Chemistry [ID Code: PIA]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
14:00-14:30	PIA/K-01	Prof. Dr. Iftikhar Ahmad	University of Malakand		01
14:30-14:45	1.	Ali Umar	Department of Chemistry, University of Malakand	Removal of Diamond Green G Dyes from Aqueous Solution by Trimetallic (Cu-Ni-Zn-BTC) MOF	11
14:45-15:00	2.	Ata Ur Rahman	Department of Chemistry, University of Malakand	Synthesis and Characterization of silica monolith particles and their modification to RPLC stationary Phase	12
15:00-15:15	3.	Atta ul Haq, Dr.	Government College University Faisalabad, Pakistan	Nickel oxide nanoparticles grafted on graphene oxide (NiO/GO) as photocatalyst for degradation of Clothianidin under UV/visible light irradiation	13
15:15-15:30	4.	Barkat Ullah, Dr.	Department of Chemistry, University of Malakand	Synthesis and Adsorption Studies of Gellan Gum Grafted Polyacrylic Acid Hydrogels	14
15:30-15:45	5.	Hanif Subhan, Dr.	Department of Chemistry, University of Malakand	Sodium Alginate Grafted Hydrogel for Adsorption of Methylene Green and Use of the Waste as an Adsorbent for the Separation of Emulsified Oil	15
15:45-16:00	6.	Hassan Imran Afridi, Dr.	National Center for Excellence and Analytical Chemistry, University of Sindh, Jamshoro - Pakistan	Essential elemental levels with Proton Pump Inhibitors in the biological samples of gastrointestinal disturbed patients residing in different cities of Sindh, Pakistan	16
16:00-16:30	REFRESHMENT BREAK				
Technical Session-1a - Physical, Inorganic & Analytical Chemistry [ID Code: PIA] (Continued)					

Technical Session-1b - Organic and Biochemistry [ID Code: OBC]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
14:00-14:30	OBC/K-01	Prof. Dr. Haq Nawaz Bhati	University of Agriculture Faisalabad, Pakistan	Treatment of Organic Pollutants by Plant Peroxidases-An Ecofriendly Approach	01
14:30-14:45	1.	Aamer Saeed	Quaid-i-Azam University Islamabad	Exploring Acyl Thiotriazinoindole Based Pharmacophores: Design, Synthesis, and SAR Studies with Molecular Docking and Biological Activity Profiling against Urease, α amylase, α glucosidase, Antimicrobial, and Antioxidant Targets	17
14:45-15:00	2.	Abdul Ghaffar Solangi, Dr.	Institute of Chemistry Shah Abdul Latif University Khairpur Sindh Pakistan	Green-Mediated Synthesis of $NiCo_2O_4$ Nanostructures Using Radish White Peel Extract for the Sensitive and Selective Enzyme-Free Detection of Uric Acid	18
15:00-15:15	3.	Abdullah Ijaz Hussain, Dr.	Government College University Faisalabad	Polyphenols: Isolation, Purification, Characterization and Evaluation of Biological Activities	19
15:15-15:30	4.	Aftab Alam, Dr.	Department of Chemistry, University of Malakand	Synthesis and characterization of biologically active flurbiprofen amide derivatives as selective prostaglandin-endoperoxide synthase II inhibitors: In vivo anti-inflammatory activity and molecular docking	20
15:30-15:45	5.	Ammara	Department of Chemistry, University of Malakand	Structure-Based Design and Synthesis of Trolox-1,3,4-Oxadiazole Hybrids with Potential Multi-Target Bioactivities	21
15:45-16:00	6.	Anoosha Sajjad	Islamia College Peshawar	Synthesis and Characterization of Iron Oxide (II, III), its Drug Conjugates with Thalidomide, and their Biological Applications	22
16:00-16:30	REFRESHMENT BREAK				
Technical Session-1b - Organic and Biochemistry [ID Code: OBC] (Continued)					

Technical Session-1c - Applied, Theoretical & Environmental Chemistry (ID: ATEC)					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
14:00-14:30	ATEC/K-01	Prof. Dr. Hassan Sher	Vice Chancellor University of Swat		02
14:30-14:45	1.	Ashfaq A. Khan	Department of Chemistry, Govt. Postgraduate College, Haripur	DNA Comet Assay for Screening of Un-irradiated and Irradiated Samples of Beans, Pulses, Tree nuts, Spices and Meats	23
14:45-15:00	2.	Farah Naz Talpur	National Centre of Excellence in Analytical Chemistry, University of Sindh	Increasing Use of Plastic Bottle Beverages in Pakistan: A Potent Source of Endocrine Disruptor Phthalates	24
15:00-15:15	3.	Fazilat Bano	University of Okara	Doping Superalkalis on Chlorine Substituted Coronene: Interactive Design Computation of New NLO Materials for Optoelectronics	25
15:15-15:30	4.	Hidayat Ullah	Institute of Chemical Sciences, Gomal University Dera Ismail Khan	Heavy metal pollution in the urban-rural interfaces: A threat to human health and ecosystem sustainability	26
15:30-15:45	5.	M.T. Saddique	National Textile University, Faisalabad, Pakistan	Synthesis of Sodium Alginate – Kernel Powder Blend Beads and their Surface Properties in Removal of Heavy Metals from Aqueous Media	27
15:45-16:00	6.	Mahwish Iqbal	University of Agriculture Faisalabad, Pakistan	Microwave Plasma: An Innovative Strategy for Enhancing Structural and Photocatalytic Properties of Silver Zirconate/GO Nanocomposite	28
16:00-16:30	REFRESHMENT BREAK				
Technical Session-1c - Applied, Theoretical & Environmental Chemistry (ID: ATEC) (Continued)					

Technical Session-2a - Physical, Inorganic & Analytical Chemistry [ID Code: PIA]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
11:00-11:30	PIA/KL-02	Prof. Dr. Tajnees Pirzada	Shah Abdul Latif University, Khairpur, Sindh, Pakistan	Comparative Studies Of Humic & Fulvic Acids Extracted From Different Sources	02
11:30-11:45	1.	Hussain Shah	Department of Chemistry, University of Malakand	A Photo-responsive Sn and Pt doped Zirconia Catalyst for the degradation of Acid Yellow-76	29
11:45-12:00	2.	Ikram Ullah	Department of Chemistry, University of Malakand	A simple 2,4-dihydroxyacetophenone based fluorescent chemosensor for detection of copper(II) ion	30
12:00-12:15	3.	Jehangir Khan, Dr.	Department of Chemistry, University of Malakand	Synthesis and Computational Study of an Optical Fluorescent Sensor for Selective Detection of Ni^{2+} Ions	31
12:15-12:30	4.	Komal Shah, Dr.	NCEAC, University of Sindh, Jamshoro	Green Synthesis of Mono and Bimetallic Nanoparticles and Their Applications	32
12:30-12:45	5.	Muhammad Ali, Dr.	Department of Chemistry, University of Malakand	Adsorptive Removal of Cetyltrimethyl Ammonium Bromide (CTAB) Surfactant from Aqueous Solution: Crossbreed Pilot Plant Membrane Studies	33
12:45-13:00	6.	Muhammad Hafeez, Dr.	University of Azad Jammu & Kashmir	Water Quality Profile of North Eastern Pakistan	34
13:00-14:00	LUNCH BREAK				

Technical Session-2b - Organic and Biochemistry [ID Code: OBC]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
11:30-12:00	PIA/KL-02	Prof. Dr. Imran Din	School of Chemistry University of the Punjab		03
11:30-11:45	1.	Aqsa Mumtaz	University of Veterinary & Animal Sciences (Jhang campus)	Hepatoprotective Potential Of Vitis vinifera Silver Nanoparticles against Acrylamide Induced Liver Damage In Rabbits	35
11:45-12:00	2.	Arifa Khanam	Department of Chemistry, Government College University Faisalabad, Faisalabad	Phenolic Profile of Seedless Ziziphus mauritiana Fruits and Leaves Extracts with In Vivo Antioxidant and Anti-inflammatory Activities: Influence on Pro-Inflammatory Mediators	36
12:00-12:15	3.	Benish Zeb	Timergara Dir lower Danwah	Bioactive profile of Ocimum americanium Antimicrobial, Antibiofilm and Antipellicule Assays	37
12:15-12:30	4.	Farwa Batool	University of Education Lahore	Determination of Phytochemical Constituents of Choro (Angelica glauca) Leaves Extracts and their Biological Studies	38
12:30-12:45	5.	Hafiz Irshadullah Khattak	Department of Pharmacy, University of Swabi, Swabi, Khyber Pakhtunkhwa, Pakistan	Computational modeling of proton pump inhibitors against 4F5S, 1IK3, and 3TOP targets: a study on advanced glycation end products	39
12:45-13:00	6.	Ijaz Ali	Department of Chemistry, University of Malakand	Synthesis and Pharmacological Screening of Thiourea Derivatives	40
13:00-14:00	LUNCH BREAK				

Technical Session-2c - Applied, Theoretical & Environmental Chemistry (ID: ATEC)					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
11:30-12:00	PIA/KL-02	Prof. Dr. Safer Ahmad	Department of Chemistry Quaid i Azam University Islamabad, Pakistan		04
11:30-11:45	1.	Mohsin Siddique	University of Sialkot	Hydrothermal Synthesis of Quaternary FeBiZn Selenide Nanocomposites for Efficient Degradation of Organic Contaminants in Aqueous Solutions	41
11:45-12:00	2.	Muhammad Imran	School of chemistry, University of the Punjab	Bismuth doped metal oxides as excellent candidates for photocatalytic and energy storage materials	42
12:00-12:15	3.	Muhammad Ismail	Department of Chemistry, University of Malakand	First principle study of PTO based porous extended conjugated polymer of high potential as a cathode material for Mg-ion batteries	43
12:15-12:30	4.	Muhammad Naeem Khan	School of Chemistry, University of The Punjab	A Study of Polystyrene and Cement Composites; their Application as a New Construction Material	44
12:30-12:45	5.	Mujtaba Ellahi	Balochistan University of Information Technology, Engineering and Management Sciences (BUITEMS). Quetta, Pakistan.	Flexible ITO Coated PET/Glass Based Thin PDLC Films using Diethyl Toluene Diamine (DETDA) Hardener	45
12:45-13:00	6.	Munawar Iqbal, Dr.	School of Chemistry, University of the Punjab, Lahore, Pakistan	Biogenic Synthesis of Zinc Oxide Nanoparticles Using NARC G1 Garlic (Allium sativum) Extract, their Photocatalytic Activity for Dye Degradation and Antioxidant Activity of the Extract	46
13:00-14:00	LUNCH BREAK				

Technical Session-3a - Physical, Inorganic & Analytical Chemistry [ID Code: PIA]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
14:00-14:30		Prof.Dr. Adnan Mujahid	School of Chemistry University of the Punjab		05
14:30-14:45	1.	Muhammad Sohail	Department of Chemistry, AIOU H-8, Islamabad	An efficient Fe2Se3/Fe2O3 Heterostructure Electrocatalyst for Oxygen Evolution Reaction	47
14:45-15:00	2.	Muhammad Tariq	NCE in Physical Chemistry, University of Peshawar	Electrochemical sensing of dopamine on metal oxides modified glassy carbon electrode	48
15:00-15:15	3.	Nazia Rafique	PARC-National Agricultural Research Centre, park road Islamabad	Optimization and validation of an analytical method for the analysis of seventy-seven pesticides in tomatoes using modified QuEChERS and LC-ESI-MS/MS	49
15:15-15:30	4.	Sami Ullah	GDC Gul Abad Dir Lower	A DFT Study of Synthetic Drug Aprocitentan: MEP, HOMO, LUMO, NBO and FUKUI FUCTION Analysis	50
15:30-15:45	5.	Shahid Khan	Department of Chemistry UOM	Synthesis of poly GG-co-AAm-co-MAA; A terpolymer hydrogel for the removal of methyl violet and fuchsin basic dyes from aqueous solution	51
15:45-16:00	6.	Shanza Mujeeb	COMSATS University Islamabad Abbottabad	Spectroscopic Studies of the Interactions of Bisphenol A with Cetyltrimethyl Ammonium Bromide	52
16:00-16:30	16:00 -16 :30 REFRESHMENT BREAK + POSTER EXHIBITION				

Technical Session-3b - Organic and Biochemistry [ID Code: OBC]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
14:00-14:30		Prof. Dr. Adeel Afzal	School of Chemistry University of the Punjab		06
14:30-14:45	1.	Imad Ali	Department of Chemistry, University of Malakand	Synthesis and Bioactivity Evaluation of 3-Ethoxy-4-Hydroxybenzaldehyde Based-Benzimidazole Derivatives	53
14:45-15:00	2.	Laiba Asif	Islamia College Peshawar	Green Synthesis, Characterization Of ZnO Nanoparticles and its Conjugates Prepared with Thalidomide and Biological Activities	54
15:00-15:15	3.	Maha Gul Zafar	University of veterinary and animal sciences Lahore ,sub campus jhang sadar	Chemical fingerprinting, In-vitro and in-silico antioxidant and anti-aging potential of Crocus sativus (Saffron)	55
15:15-15:30	4.	Muhammad Ali Shah	Department of Chemistry, University of Malakand	Synthesis, Bioactivity and Photophysical Property of Benzophenone Bis Schiff Bases	56
15:30-15:45	5.	Bilal Ahmad	Department of Chemistry, University of Malakand	Synthesis and Characterization of Nitro-Substituted Polyhydroquinoline Derivatives	57
15:45-16:00	6.	Muhammad Waqar	Department of Chemistry, University of Malakand	Synthesis, Evaluation of Biological Activities, and Molecular Modeling of Ketoprofen Derivatives	58
16:00-16:30	16:00 -16 :30 REFRESHMENT BREAK + POSTER EXHIBITION				

Technical Session-3c - Applied, Theoretical & Environmental Chemistry (ID: ATEC)					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
14:00-14:30		Prof. Dr. Muhammad Arshad	Institute of Chemistry the Islamia University of Bahawalpur		07
14:30-14:45	1.	Qaisar Khan	Johannes Gutenberg University, Mainz, Germany	Structural features, dielectric and magnetic properties Yb-ion substituted Co-Zn spinel ferrites	59
14:45-15:00	2.	Seemab Javed	Government College University Faisalabad	Alkaline Fusion Assisted Synthesis of K-Zeolite from Rice Husk for Wastewater Treatment	60
15:00-15:15	3.	Sundus Munir	COMSATS University Islamabad, Abbottabad Campus	Investigation of Optical Properties and Wettability of Chitosan/Silica Composite Films	61
15:15-15:30	4.	Syed Muhammad Saqib Nadeem	Public Sector Organization I-10/2, Islamabad.	Reverse Osmosis Technology: A Possible Solution to Global Water Scarcity	62
15:30-15:45	5.	Tajamal Hussain	School of Chemistry, University of the Punjab, Lahore	Single-Step Synthesis of Co/Ni/Cu Trimetallic Nanoparticles and Photocatalytic Purification of Water	63
15:45-16:00	6.	Umar Farooq	School of Chemistry, University of the Punjab, Lahore	Fabrication of Co3O4 and Co3O4-Cu-BTC based Electrochemical Sensor for Voltammetric Determination of Toxic Cadmium ions	64
16:00-16:30	16:00 -16 :30 REFRESHMENT BREAK + POSTER EXHIBITION				

Technical Session-4a - Physical, Inorganic & Analytical Chemistry [ID Code: PIA]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
09:00-09:30		Prof.Dr. Muhammad Zaman Ashraf	Rawalpindi Women University Islamabad	Tyrosinase Enzyme a Promising Target for the Design and Synthesis of Anti-Melanogenic Agents	08
09:30-09:45	1.	Umar Wahab, Dr.	Department of Chemistry, University of Malakand	Chemo-selective Hydrogenation of Carbonyl Compounds over Bimetallic Catalysts	65
09:45-10:00	2.	Sadia Ata, Dr.	School of Chemistry, University of the Punjab, Lahore	Innovative Ni-Based Metallic Foams: A Pathway to Sustainable Hydrogen Production through Water Splitting	66
10:00-10:15	3.				
10:15-10:30	4.				
10:30-10:45	5.				
10:45-11:00	6.				
11:00-11:15	7.				
11:15-11:30	8.				
11:30 - 12:00	CLOSING SESSION & Farewell to the Guests				

Technical Session-4b - Organic and Biochemistry [ID Code: OBC]					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
09:00-09:30		Prof. Dr. Shahzad Ali Shahid Chatha	Government College University Faisalabad	Zero Waste Economy through Upcycling of Industrial Wastes	09
09:30-09:45	1.	Qudsia Jalil	Department of chemistry, Islamia College, University Peshawar	Synthesis, Characterization of Biocompatible Iron Oxide Nanoparticles Drug Conjugates With Thalidomide: An Alternate to Boost the Anti-inflammatory and Alkaline Phosphatase Assays	67
09:45-10:00	2.	Rehan Ullah	Department of Chemistry, University of Malakand	Dicarboxamide Derivatives of Salicylic Acid: Synthesis, Characterization and Biological Activities	68
10:00-10:15	3.	Saima Malik	Institute of Chemistry, Shah Abdul Latif University Khairpur	Characterization of humic acid from Thar coal mines Sindh, Pakistan	69
10:15-10:30	4.	Salman Zafar	Institute of Chemical Sciences, University of Peshawar	Microbial Models for *in vivo* Drug Metabolism	70
10:30-10:45	5.	Shabir Ahmed Dharejo	Shah Abdul Latif University, Khairpur, Sindh, Pakistan	Characterization and biofabrication of isolated silver nano particles with humic acid and their role against test pathogens causing skin infections	71
10:45-11:00	6.	Sulaiman	Department of Chemistry, Islamia College University, Peshawar	Synthesis of zinc oxide based etoricoxib and montelukast nanoformulations and their biomedical applications	72
11:00-11:15	7.	Syed Faheem Askari Rizvi	School of Basic Medical Sciences, Lanzhou University, Lanzhou 730000, Gansu, P. R. China	Novel pH-Responsive Peptide-Paclitaxel Conjugate with Improved Therapeutic Potentials against Glioblastoma	73
11:15-11:30	8.	Luis Menéndez-Arias	Centro de Biología Molecular Severo Ochoa (Consejo Superior de Investigaciones Científicas & Universidad Autónoma de Madrid), c/ Nicolás Cabrera 1, 28049 Madrid, Spain	HIV-1 replication: fidelity, drug resistance and unexploited antiviral targets	74
11:30 - 12:00	**CLOSING SESSION & Farewell to the Guests**				

Technical Session-4c - Applied, Theoretical & Environmental Chemistry (ID: ATEC)					
Time	No.	Name	Affiliation	Talk Title	Abstract on Page
09:00-09:30		Prof. Dr. Humaira Yasmeen Gondal	Institute of chemistry, University of Sargodha	Functionalization in Organic Synthesis: Key to Unfold Versatile Applications	10
09:30-09:45	1.	Waqas Ahmad	Institute of Chemical Sciences, University of Peshawar	Extraction of Cu from copper smelting through leaching using organic and inorganic lixiviants	75
09:45-10:00	2.	Tanzeela Ahmad Shah	Department of Chemistry, University of Malakand	Experimental and Computational Profiling of Novel Bis-Schiff Base Derivatives Bearing α-Naphthalene Moiety as Potential Tyrosinase Inhibitors	76
10:00-10:15	3.	Weenghar Ali Chandio	Institute of Chemistry , Shah Abdul Latif University Khairpur, Sind Pakistan	Effects of Zinc Oxide Nanoparticles coated with naturally occurring Humic Acid on Germination of Seeds	77
10:15-10:30	4.	Muhammad Usman	Department of Chemistry, University of Malakand	Synthesis, Characterization, Enzyme Inhibition and Molecular Docking Studies of Benzothiazole Derivatives Bearing Alkyl Phenyl Ether Fragments	78
10:30-10:45	5.	Sajjad Ur Rahman	Department of Chemistry, University of Malakand	Novel Acyl Hydrazide Derivatives of Polyhydroquinoline as Potent Anti-Diabetic and Anti-Glycating Agents: Synthesis, In Vitro α-amylase, α-glucosidase Inhibition and Anti-glycating activity with Molecular Docking Insights	79
10:45-11:00	6.	Muhammad Ayaz	Department of Chemistry, University of Malakand	Bio-Oriented Synthesis of Ibuprofen-Clubbed Novel Bis-Schiff Base Derivatives as Potential Hits for Malignant Glioma: In Vitro Anticancer Activity and In Silico Approach	80
11:00-11:15	7.				
11:15-11:30	8.				
11:30 - 12:00	CLOSING SESSION & Farewell to the Guests				

List of Poster Presentations

Plenary Lecture- 01(Virtual)

Prof. Dr. Atta Ur Rahman

Patron Chemical Society of Pakistan

Plenary Lecture-02

Dimensional Tailoring of hybrid perovskites for efficient and stable solar cells

Prof. Dr. Mohammad Khwaja Nazeeruddin

Group for Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, Ecole polytechnique fédérale de Lausanne (EPFL), CH-1951 Sion, Switzerland

Organic-inorganic lead halide perovskites have shown impressive power conversion efficiency (PCE) in a range of solar cell architectures.1-2 Despite the multiple ionic compositions that have been reported so far, the presence of organic constituents is an essential element in all the high efficiency formulations, with the methylammonium (MA) and formamidinium (FA) cations being the sole realistic options available to date. In this study, we demonstrate a novel three dimensional (3D) perovskite with improved material stability as a result of the incorporation of an alternative organic cation, guanidinium, into the MAPbI3 crystal structure.3 The new MA1-xGuaxPbI3 perovskite shows enhanced thermal stability and intrinsically new structural and optoelectronic properties. This allows for stable and high-power conversion efficiencies over 20%, a fundamental step within the perovskite field.

Plenary Lecture-03

Sustainable and Inclusive Drug Discovery at the Interface of Chemistry and Biology – *Examples of Our Recent Work*

Prof Dr. Iqbal Choudhary

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Sustainable drug discovery and development is based on the principles of the use of renewable resources, and green chemistry methods. Nature-based discovery of drugs against prevailing and emerging diseases is sustainable and inclusive. Our work in the past two decades has been focused on the discovery of new drug leads from medicinal plants, as well as synthesis of bioactive analogs by biocatalytic transformations. We have been working largely at the interface of chemistry and biology for the discovery of chemical constituents from plants used in traditional medicines, as well as for designing of new biotransformed products with therapeutic potential. This has resulted in the identification of several novel drug leads against various therapeutic targets. Emphasis has been on the discovery of natural products, and their analogs against chronic disorders, including cardiovascular, cancer, diabetes, inflammatory diseases, and Alzheimer's and Parkinson's diseases. Novel analogues of existing drugs such as tibolones (postmenopausal osteoporosis), exemestane (anti-cancer drug), medrysone (anti-inflammatory agent) and many others were synthesized using biotransformation tools. Thus potent anti-inflammatory, and anti-cancer agents were identified as lead molecules. Furthermore, inhibitors of key enzymes related to several diseases were also identified. During this presentation, some recent examples of our studies highlighting the translational potential of bioactive natural products, and biotransformation against non-communicable chronic diseases will be presented.

Plenary Lecture-04

Supramolecular Approach in Delivery System

Prof. Dr. M. Raza Shah

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Macrocycles has been the subject of great interest due to its unique topology, binding sites and high selectivity towards analytes due to geometrically controlled cavity. A series of macrocycles bearing electron acceptors and electron-donor groups with high pH-sensing behavior were synthesized in good yields. The structures of all macrcycles and their precursors were established through 1D and 2D NMR spectroscopy, mass spectrometry, FT-IR, UV-visible spectroscopy and elemental analysis. Fluorescence-enhancement and quenching behavior of the macrocycles and their pre-cursors were utilized for the detection and distinction of environmentally important analytes in the drinking water resources of Karachi in one hand and biological matrix on the other hand. UV-Visible spectrophotometric titrations, cyclic volatmmetry were effectively used for on-off changes experienced upon binding of analytes with macrocycles. Analysis of the crystal structures of the macrocycles revealed their preference for well-preorganized bent-sheet conformations, both as free receptors and their complexes with anions.

Plenary Lecture-05

Synthesis, Characterization and application of new materials for enrichment and determination of organic and inorganic species of environmental importance

Prof. Dr. Mohammad Rasul Jan

Professor Emeritus, Institute of chemical Sciences University of Peshawar

The overexploitation for natural resources has led to many issues including the availabilities of the badly needed nonrenewable resources. This has necessitated the search for resource recovery for reuse in commercial applications. There is also a continuous challenge for determination of trace chemical at affordable cost to ensure safety of consumer product including potable water. To come up to these challenges scientist are investigating new materials for resource recovery, enrichment and determination at trace levels. A variety of novel graphene based nanocomposite modified and unmodified were synthesized and characterized using FTIR, SEM and EDX for functional groups, morphology and elemental analysis respectively. These nano composites were used for simultaneous pre-concentration of trace elements such as Pb, Cu, Ni and Co prior to its determination by flame atomic absorption spectroscopy. Nano composite were also tried for solid phase and liquid liquid micro extraction of emerging pharmaceutical pollutants and aromatic amines. Various parameters, effecting sorption efficiency were investigated. The details of our investigations will be presented and discussed.

Plenary Lecture 06

Developing Framework and Ecosystem for the technology transfer for the economic growth in Pakistan

Najeebullah

In the era of Industry 4.0, traditional methods in agriculture and industry are struggling to keep pace with rapid economic advancements. This talk explores the concept of a knowledge-based economy and presents a framework for leveraging it to drive Pakistan's economic growth. Data was collected from various government departments, including the Ministry of Science and Technology, the Higher Education Commission, venture capital firms, and other financial entities within the ecosystem and industry. The research reveals that Pakistan significantly lags in three key pillars of a knowledge-based economy. Government spending on research is notably insufficient, ranking among the lowest in the region. Research institutes are largely non-functional and require comprehensive restructuring. The capital landscape remains underdeveloped, necessitating substantial government support. Furthermore, the quality of education and research in universities, along with university rankings essential for fostering innovation, require substantial improvement. This talk will provide recommendations categorized into four sections: addressing university challenges and outlining a strategic path forward, establishing an effective capital model for the financial landscape, restructuring the Ministry of Science and Technology, and defining the government's roles and responsibilities in driving this critical transition.

Plenary Lecture 07

Heterogeneous Catalytic Hydrogenation

Bagher Eftekhari-Sis

University of Maragheh, Iran

Hydrogenation is one of the oldest application methods applied in the laboratory and dates back to the 1900s. Heterogeneous catalytic hydrogenation (HCH) play a very important role in the synthesis of many organic molecules both in research laboratories and in industry. In this chapter, HCH reactions of organic compounds containing many different substituents such as alkenes, alkynes, carbonyl compounds, N-heterocycles and nitroarenes are comprehensively discussed. Additionally, the role of HCH in reductive amination reactions, which is another application of catalytic hydrogenation reaction, was demonstrated.

Keywords: Heterogeneous, Catalytic Hydrogenation

Plenary Lecture 08

Synthesis and Characterization of new 2-bromo-3-(hetero/aryl)amino-1,4-naphthoquinone derivatives

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Quinones are abundantly found in nature and have an importance for the cell's life cycle. The quinone-containing compounds have a wide range of pharmacological activities, such as anticancer, antiviral, and anti-neurodegenerative activities, etc. [1] The redox feature of 1,4- quinone plays a significant role in the pharmacological effectiveness [2]. 1,4-naphthoquinones among the quinone-bearing compounds are the most significant members [3]. These compounds are used to manufacture many important molecules with medicinal and industrial interests. These compounds can be modified by nucleophilic substitution reaction of various nucleophiles with sulfur, oxygen, and nitrogen with 2,3-dichloro and 2,3-dibromo-1,4- naphthoquinone or 1,4-naphthoquinone core for accessing the molecules with promising biological activities [4].

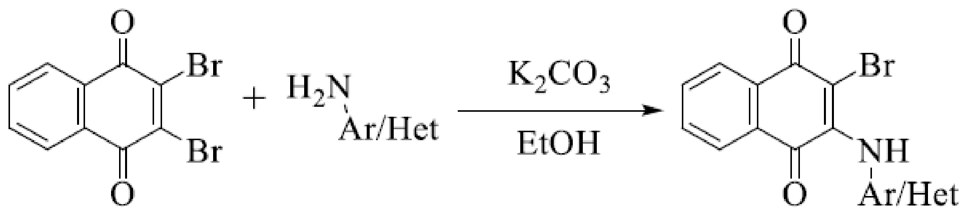

Fig. 1. The substitution reaction of 2,3-dibrom-1,4-naphthoquinone with aromatic or heteroaromatic amines

In this study, the nucleophilic substitution reaction (**Fig. 1**) of various aromatic and heteroaromatic amine derivatives was carried out in ethanol with K2CO3 as a base. The products were characterized by high-resolution mass spectrometry, FT-IR, ^{1}H, and ^{13}C NMR methods. These compounds may exhibit a range of biological actions, which will be evaluated soon.

Keynote Lecture 1a

Prof. Dr. Iftikhar Ahmad
Meritorious Professor, University of Malakand

Keynote Lecture 1b

Treatment of Organic Pollutants by Plant Peroxidases-An Ecofriendly Approach

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Development of environmentally sustainable processes is a challenging task for the current bioeconomy. In this direction, the use of biocatalysts, enzymes, in various processes is considered as an ecofriendly approach. The stability, activity and specificity of enzymes are the fundamental parameters that are required to develop enzymes for their optimal applications in various industrial processes. Peroxidases, one of the key antioxidant enzymes, are widely distributed in nature and catalyze oxidation of various electron donor substrates concomitant with the decomposition of H_2O_2. The non-animal plant peroxidases (class III peroxidase) are involved in various essential physiological processes of plant growth and development throughout their life cycle. In view of the capability of peroxidases to catalyze the redox reaction for a wide range of substrates, they are considered as one of the important enzymes from the point of view of their various medicinal, biochemical, immunological, biotechnological, and industrial applications. Enzymatic treatments have attracted much attention as cost effective and environment friendly techniques for detoxification of dye contaminated industrial effluents. Use of plant peroxidases for the remediation of dyes has demonstrated promising results indicating that these are cost effective and ecofriendly systems.

Keywords: Biocatalysts, Peroxidases, Bioremediation, Ecofriendly, Sustainable

Keynote Lecture 1c

Prof. Dr. Hassan Sher
Vice Chancellor University of Swat

Keynote Lecture 2a

Comparative Studies of Humic & Fulvic Acids Extracted from Different Sources

Tajnees Pirzada

Institute of Chemistry, Shah Abdul Latif University Khairpur, Sind, Pakistan

There is very less information on the chemical and spectral properties of humic substances obtained from various natural organic sources. Humic substances are ubiquitous and are found whenever organic matter is undergoing decomposition. Structurally ill-defined humic substances consist of aromatic ring structures with aliphatic side chains, mainly oxygen containing functional groups, “bridge” units Humic acid (HA) and (FA) are used in different aspects of life, in disorders such as Alzheimer's disease, respiratory tract infections, cancer, fatigue, heavy metal toxicity, allergies, and preventing a condition in which the body tissues do not receive enough oxygen (hypoxia) and commonly FA applied on the skin for eczema and to carry out important chemical reactions in the body to boost immune system. Humic substances are also important for plants as they help to make nutrients in the soil available to the plants, in drought conditions. Fulvic acid contained more functional groups than humic acid extracted from all organic sources, including carboxyl and phenolic-OH groups. According to the spectroscopic analysis, humic acid has lower E4/E6 ratio values than fulvic acid. UV-Vis spectra revealed that humic substances contained aliphatic as well as aromatic components. FTIR spectra revealed that humic and fulvic acids contain aliphatic CH, hydroxy, and carboxyl groups with varying values depending on the organic sources. This research also confirmed the wide composition of organic substances and humic substance variations in different sources and the influence of extraction conditions. Therefore, in future research of natural organic matter will be focused on specifying parameters for standardization and development of bioactive substances.

Keywords: Humic acid, Fulvic acid, spectroscopic analysis, comparative studies

Keynote Lecture 2b

Molecularly Imprinted Polymer Film on Silica Particles for Recognition of Environmental Toxic Amines

Dr. Muhammad Imran Din

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This research focus on the synthesis of surface-molecularly imprinted polymeric materials for the recognition of environmental toxic amines, using a grafting methodology. Silica particles serve as the underlying substrate onto which a molecularly imprinted polymer film is deposited. The synthesis of uniformly distributed silica particles was carried out by hydrolysis of the precursor. The polymerization process involves the utilization of acrylic based polymer system. The resultant surface-grafted polymer is subjected to characterization using UV/Vis spectroscopy to evaluate its recognition capabilities towards amines. Rebinding studies involving polymer-template interactions are studied wherein surface molecular imprinted particles demonstrated a substantially enhanced recognition towards amines. Furthermore, the class selectivity of surface-imprinted particles is also assessed. Lastly, the reusability of the developed product is investigated, revealing that regenerated imprinted particles exhibited retention of over 80% of their recognition features compared to freshly prepared counterparts. The current study demonstrates the suitability of surface imprinted silica particles as potential affinity material for removal of toxic amines thus, providing a facile solution to treat wastewater samples.

Keywords: Amines; Silica; Molecular Imprinting; Wastewater.

Keynote Lecture 2c

Physics and Chemistry of Electrochemical Impedance Spectroscopy

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Electrochemical impedance spectroscopy (EIS) is one of the several electrochemical techniques being used for last five to six decades primarily to understand the kinetics and mechanism of charge transfer or allied processes under investigation. EIS is a highly powerful method for the detailed and in-depth analysis of an electrochemical system. With the advancement of technology and with the establishment of 'material chemistry' as a full-fledged discipline, the utilization of EIS has increased considerably. Further, the applications of EIS in the understanding of the different properties of a material, particularly the energy materials, is attaining popularity day by day. Considering the importance of method at its own and its growing applications this presentation is divided into three parts. (a) The basis of EIS will be presented which deals overwhelmingly the physics (and a bit of electronics!) behind the technique. The links with the fundamentals of electrochemistry will also be shared. (b) In this part the well-established analyses of EIS will be discussed along with their experimental set-up and the outputs. How are the fundamental parameters obtained and how can they be utilized to acquire possible information? This question will be addressed while discussing the chemistry aspects of the EIS. (c) Lastly some case studies will be shared where the EIS has been successfully used to investigate and interpret the property of interest. Though it is a difficult task to get the attention of the audience for this complex methodology however, it would be interesting and aspiring for those who are already on it or in search of its understanding from scratch.

Keywords: Impedance; Electrochemistry; Frequency; Experimental setup; Energy materials.

Keynote Lecture 3a

Unlocking the Potential of Ready to Use Polymers for Imprint-Based Electrochemical Sensors

Adnan Mujahid

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This investigation centers on elucidating molecular imprinting phenomena within ready to use polymers for evaluating their potential utility in electrochemical sensor development. The template molecule was incorporated into a clear polymer solution for the production of molecularly imprinted polymer (MIP) coatings, which were subsequently spin-coated onto interdigitated capacitors (IDCs). These coated IDCs were then subjected to standard analyte solutions of varying concentrations, and their corresponding capacitance responses were recorded across differing frequencies. Analogous procedures were conducted for non-imprinted polymer (NIP) coatings in conjunction with IDCs, while uncoated devices were also subjected to testing. Structural characterization of both MIPs and NIPs was conducted via Fourier transform infrared spectroscopy (FTIR), revealing comparable polymer backbones. The MIP-coated sensor exhibited a linear signal response, attributable to the specialized interaction sites engendered by molecular imprinting, whereas the NIP-coated device evinced substantially diminished response. The MIP sensor demonstrated the highest sensitivity comparing to NIP moreover, the MIP sensor exhibited markedly heightened selectivity toward target analyte in comparison to other interfering analytes, whereas the NIP counterpart manifested non-specific interactions. This study underscores the applicability of ready to use polymers for facilitating highly sensitive, selective, label-free, and expeditious electrochemical sensing modalities.

Keywords: Molecular Imprinting; Polymers; Sensors; Electrochemical.

Keynote Lecture 3b

Group-Selective Electrochemical Sensors for Water Quality Assessment

Adeel Afzal

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Industrial effluent discharge is one of the leading causes of water pollution, introducing hazardous substances into aquatic ecosystems and posing significant threats to both environmental integrity and public health. Among these pollutants, organic dyes, particularly anionic or acid dyes, are widely used in industries such as textiles, plastics, and paper production. Their release into water bodies leads to contamination that is harmful to both aquatic life and human populations. However, the challenge of continuous monitoring and regulation of these pollutants is exacerbated by the impracticality of identifying and measuring individual contaminants in industrial wastewater. Current methods for water quality monitoring often require sophisticated instrumentation and labor-intensive processes that are neither scalable nor cost-effective for industrial applications. In response to this issue, we have developed an innovative group-selective electrochemical sensing platform specifically designed for the large-scale detection of anionic dyes in industrial effluents. This approach leverages pencil electrodes modified with a composite of vanadium-doped graphitic carbon nitride nanosheets and recycled polystyrene (PS/V-gCN), providing an economically viable and environmentally sustainable solution. The use of recycled polystyrene as a substrate not only reduces material costs but also supports waste valorization, aligning the sensor's development with principles of green chemistry and sustainability. The PS/V-gCN-modified sensors demonstrate exceptional performance characteristics, with high sensitivity in detecting key anionic dyes such as Erichrome black T (EBT), methyl orange (MO), and Congo red (CR). These dyes, known for their wide industrial use and environmental persistence, were detected across various aqueous media, including pure solutions, mixed dye systems, and complex surface water samples. The sensors achieved impressive sensitivity values ranging from 0.44 to 1.16 $\mu A\ cm^{-2}\ nM^{-1}$, with detection limits reaching sub-nanomolar levels (<1 nM). This high sensitivity underscores the capability of the PS/V-gCN sensors to detect trace levels of pollutants, crucial for early intervention and mitigation efforts. Furthermore, the sensors exhibited strong group selectivity, effectively distinguishing between anionic and cationic dyes. While the PS/V-gCN sensors demonstrated high responsiveness to anionic dyes, their response to cationic dyes, such as methylene blue (MB) and rhodamine B (RhB), was significantly reduced. This group selectivity is a critical advantage, as it allows for the targeted monitoring of specific pollutant classes without interference from other dye types commonly found in industrial wastewater. The electrochemical techniques employed, including cyclic voltammetry (CV), differential pulse voltammetry (DPV), and electrochemical impedance spectroscopy (EIS), further validated the robustness of the sensor's performance. These methods enabled precise measurements of the electrochemical properties of the modified electrodes, ensuring both accuracy and reproducibility in detecting pollutants under varying environmental conditions. Our study highlights the potential of utilizing waste-derived materials, such as recycled polystyrene, in conjunction with advanced nanomaterials like vanadium-doped gCN to develop sensitive, reliable, and scalable sensors for environmental applications. By integrating waste management with pollutant detection, this work not only addresses water quality monitoring challenges but also contributes to sustainable development goals related to pollution control and resource conservation.

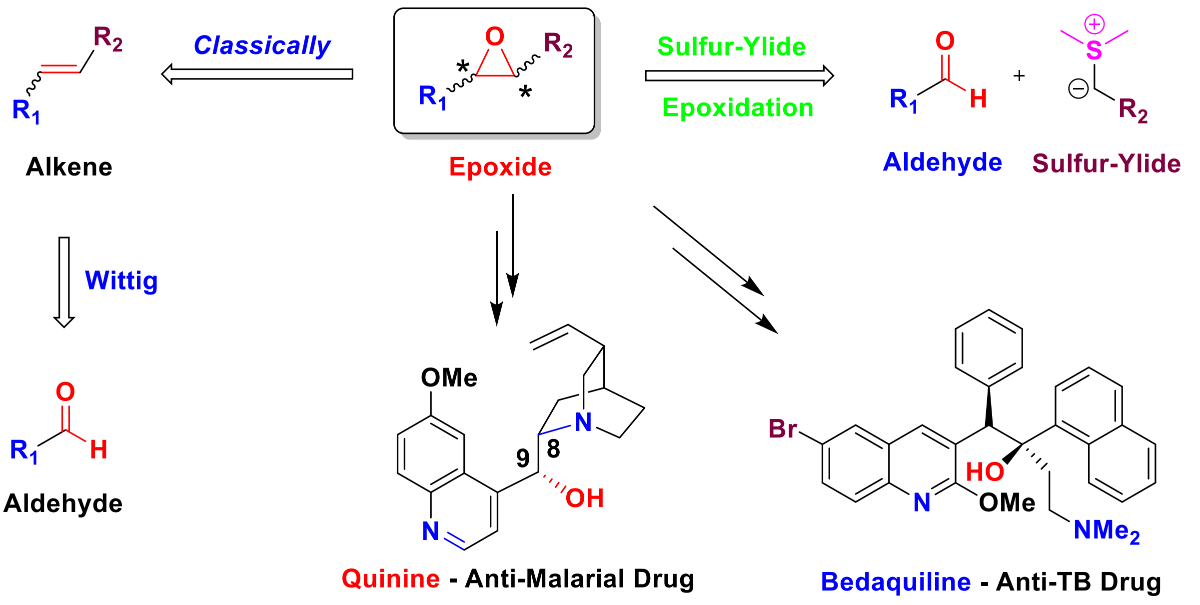
Keywords: Chemical sensors; Electrochemistry; Anionic dyes; Water quality.

Keynote Lecture 3c

Sulfur-Ylide Epoxidation in Asymmetric Syntheses of Drugs

Prof. Dr. Muhammad Arshad
Institute of Chemistry the Islamia University of Bahawalpur

Epoxides are noteworthy precursors in organic synthesis due to the presence of two contiguous chiral centres and facile transformations to a wide range of functionalized molecules possessing pharmacological significance, e.g., 1,2-diols, carbonyls, amino-alcohols etc. Numerous methods have been discovered for constructing **epoxides** (*Sharpless, Jacobsen, Shi etc.*), primarily *via* oxidation of an alkene, which, in turn is typically obtained from corresponding carbonyl compound, usually aldehyde through **Wittig** olefination. However, **the sulfur-ylide epoxidation**,[1] provides a complimentary route to **epoxides** directly from aldehydes (Scheme below). A range of chiral sulfides has been successfully employed for the asymmetric syntheses of **epoxides** through *sulfur-ylide epoxidation* methodology. Few of these sulfides have delivered high levels of diastereo- and enantioselectivities (>95% d.e. & e.e.) for **epoxide** formation.[2] Isothiocineole is one of the most successful chiral sulfide, which was afforded in single step from inexpensive and readily available starting materials like, limonene, sulfur and γ-terpinene. It was employed in the asymmetric synthesis of complex cinchona alkaloids **quinine** (*anti-malarial drug*) and its (C-8, C-9) epimer **quinidine** (*chiral ligand and catalyst*).[3] Recently, we have effectively applied this chiral sulfide for the asymmetric synthesis of a potent anti-TB drug named **bedaquiline** comprising nine steps from commercially available starting materials, which is the shortest synthesis of this drug.[4]



Keynote Lecture 4a

Prof. Dr. Muhammad Zaman Ashraf

Rawalpindi Women University Islamabad

Tyrosinase Enzyme a Promising Target for the Design and Synthesis of Anti-Melanogenic Agents

The metalloenzyme tyrosinase is a binuclear copper containing enzyme catalyzes L-tyrosine to L-3,4-dihydroxyphenylalanine (L-DOPA) and further oxidation of (L-DOPA) to dopaquinone which then transformed through several reactions into brown to black melanin.Tyrosinase is also responsible for the production of neuromelanins. The abnormal production of melanin results in Melasma, post-inflammatory hyperpigmentation (PIH), Parkinson's and other neurodegenerative diseases.Thus, it is in great need of developing new tyrosinase inhibitors without causing adverse reactions. Previous reports confirmed that presence of hydroxy substituted phenyl ring is considered to be important in tyrosinase inhibitory activity. The natural phenolic antioxidants have been selected to design and synthesize their derivatives as tyrosinase inhibitors. The computational and wet lab approaches have been utilized to get highly potent tyrosinase inhibitors. The drug development strategies through enzyme based assay particularly tyrosinase inhibitors have been established. The designed and synthesized compounds inhibitory effects on mushroom tyrosinase have been evaluated and kinetic mechanism of the potent derivatives was also determined. The docking studies of synthesized analogues have also been performed against tyrosinase protein to compare the binding affinities with IC_{50} values.We are able to find out a derivative which is thousand times more active than the standard tyrosinase inhibitor (Kojic acid). The cytotoxicity and cell based tyrosinase inhibition studies of highly potent derivatives have also been performed. These derivatives also exhibited better tyrosinase inhibitory activity in murine skin melanoma (B16F10) cells.

Keynote Lecture 4b

Zero Waste Economy through Upcycling of Industrial Wastes

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Deserted growth in urbanization and industrialization is generating huge amounts of solid waste. Fly ash: a solid industrial waste is key player of smog and climate change. It has been recognized as leachate pollutant and human carcinogen. Its dumping can be detrimental for soil fertility and ground water as well as financial liability. The most attractive and sustainable mitigation of fly ash waste is its upcycling for the synthesis value added materials. Synthesis of fly ash-based zeolites as value-added material is an economical and sustainable approach. In this work a variety of fly ashes from boiler plants of different industries were used for the synthesis of fly ash based active zeolites. Fly ash based zeolites and zeolite synergized photo-catalysts prepared by conventional and advanced curing techniques were characterized by state-of-the-art analytical techniques like; XRD, SEM, FTIR, ICP-OES and CEC and investigated for their wastewater treatment potential, Keeping in view the findings of these investigations, it is very reasonable to conclude that recycling of fly ash waste for wastewater treatment is a positive move towards achieving a sustainable green technology with zero waste economy.

Keywords: Fly ash, Synthesis, Zeolites, Wastewater treatment

Keynote Lecture 4c

Functionalization in Organic Synthesis: Key to Unfold Versatile Applications

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Abstract: Functionalization involves the strategic introduction, modification, or transformation of functional groups in organic molecules, enabling the development of structurally complex compounds with desired chemical and physical properties. The current talk will cover our efforts towards development of new task-oriented organic molecules, in the field of enantioselective organocatalysis and chiral recognizing agent. In first part, development of a highly efficient bifunctionalized amino catalyst will be explained to access structurally diverse ß-indolyl ketones in high yields (up to 91%) and excellent enantioselectivity (enantiomeric ratio up to 98:2). In the second part, investigation on synthesis and applications of ILs as chiral shift agents for the chiral recognition of racemic mixtures of Mosher's acid potassium salts will be discussed. Discussion will cover supramolecular interactions between salt and H–C2 of chiral benzimidazolium cation are responsible for the chiral recognition, as demonstrated by experimental evidences.

Removal of Diamond Green G Dyes from Aqueous Solution by Trimetallic (Cu-Ni-Zn-BTC) MOF

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Trimetallic (Cu-Ni-Zn-BTC) MOF was synthesized using the solvothermal method. Then it was characterized by SEM, FTIR, TGA, Zeta sizer Zeta potential, and BET analysis. The results confirm the synthesis of desired MOF and its suitability for adsorption application. The synthesized MOF particles were utilized for the adsorption of Diamond Green G dye from an aqueous medium. Various experimental parameters like adsorbent dosage, pH, temperature, and contact time were systematically optimized for the enhancement of adsorption effectiveness. Various kinetic and isotherm models were applied to the adsorption experimental data. Kinetic data analysis revealed that the present adsorption process followed a pseudo-second-order model, confirming the chemisorption nature of the ongoing adsorption process. On the other hand, the best-fitted isotherm model was the Langmuir isotherm model, indicating monolayer adsorption with a maximum adsorption capacity of 434 mg/g at 333 K temperature. Thermodynamic studies revealed that the adsorption process was endothermic with an enthalpy change (ΔH) of 14.76 kjmol^{-1}and an entropy change (ΔS) of 53 jmol^{-1}K^{-1}. Gibbs free energy (ΔG) was negative at all experimental temperatures and with an increase in temperature, the magnitude of Gibbs free energy decreased suggesting the spontaneous nature of the adsorption process. In the regeneration study, the particles were treated with various eluents and were utilized for many cycles. This study verified the structural stability and performance and showed its potential for reuse in industrial applications.

Synthesis and Characterization of silica monolith particles and their modification to RPLC stationary Phase

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A particle based silica monolith particle has been synthesized using tetraethyl orthosilicate (TEOS) as a precursor by a well-known Sol-gel protocol followed by soft grinding and calcination. Highly porous and mechanically stable silica particles were produced as a result of the carefully regulated hydrolysis and condensation reactions used in the synthesis process. Silica particles were used as the base material in the creation of stationary-phase medium. After synthesis, these particles are reacted with (3-aminopropyle) trimethoxysilane, followed by initiator, Sodium diethyl thiocarbamte attachment. The organic polymers consisting of styrene and EGDMA were immobilized on the surface of initiator bound silica monolith particles using a well-known reversible addition-fragmentation chain transfer polymerization (RAFT) protocol. The protocol of RAFT polymerization was optimized to get the proper thickness of polymers layer at the surface of silica monolith particles. A highly repeatable methodology for silica monolith particle modification has been established, with great repeatability for both particle and pore diameters. The synthesized co-polymer bound silica monolith particles were characterized through SEM-EDX (scanning electron microscopy, Energy dispersive X-ray), Fourier transform infrared spectroscopy (FTIR), and proton NMR.

Keywords: RPLC, silica monolith, Stationary phase, Chromatography

Nickel oxide nanoparticles grafted on graphene oxide (NiO/GO) as photocatalyst for degradation of Clothianidin under UV/visible light irradiation

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In the present work, the synthesis of NiO nanoparticles was carried through green synthesis by using extract of peels of green peas (*Pisum Sativum*). Graphene oxide was prepared through modified Hummer's method and the graphene oxide/nickel oxide nanocomposite was synthesized by ultrasonication method. The prepared nanocomposite was characterized by different techniques including XRD, FTIR and SEM. The FTIR analysis confirmed the functional groups in the prepared NiO/GO nanocomposite. Different experimental parameters such as pH, dose of catalyst, agitation rate, initial pesticide concentration and temperature were studied for the maximum degradation of clothianidin in aqueous solution. By adjusting different temperature range from 303 to 353 K, the maximum degradation was observed at 333 K, which is 78.51%. The degradation rate is increased with increase amount of dose of catalyst and maximum degradation of 92% is observed at 1g of catalyst. The maximum degradation was observed at pH 3. However, after pH 3, the degradation was decreased continuously. The concentration of stock solution of 10 ml showed maximum degradation. Furthermore, the synthesized NiO/GO nanocomposite from green route provided best economical alternative for pesticide degradation.

Keywords: Clothianidin; Photocatalytic degradation; NiO nanoparticles; Graphene Oxide; NiO/GO nanocomposite

Synthesis and Adsorption Studies of Gellan Gum Grafted Polyacrylic Acid Hydrogels

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Gellan Gum grafted poly-Acrylic Acid (GG-g-pAAc) hydrogels of different composition were synthesized by changing the concentration of Gellan Gum with respect to Acrylic Acid and were characterized through Scanning electron microscopy (SEM), thermogravimetric analyzer (TGA) and Fourier transform infrared (FTIR). FTIR showed the grafting of Gellan Gum into the network of polyacrylic acid confirming GG-g-pAAc formation. SEM analysis provided information about the channels, pores and sites for adsorption in the synthesized hydrogels particles. The thermogravimetric analyzer (TGA) shows that the mass of synthesized hydrogels decreases with the increase in temperature. With an efficiency of 96%, Basic Orange-2 dye was successfully removed from wastewater using synthesized hydrogels as an adsorbent. The adsorption parameters were calculated using a number of different kinetic models. According to the findings, the pseudo-2nd order kinetics model best suited to the kinetics data, while the Langmuir isotherm provided the most comprehensive explanation of the process of adsorption. Basic Orange-2 dye was removed to the greatest extent (257.5 mg/g) after 2 hours at 293K. Additionally, the results showed that the adsorption process on synthesized hydrogels was exothermic because the values of ΔH were found to be negative (ΔH = -13.2, -219.4 and -12.9 kJ/mol for pAAc, 10%GG-g-pAAc and 20%GG-g-pAAc respectively). The adsorption process in this study is spontaneous, as it is clear from the negative values of ΔG, (ΔG = -8.2, -214.4 and -7.947 kJ/mol for pAAc, 10%GG-g-pAAc and 20%GG-g-pAAc at 293K respectively). The adsorption process on synthesized hydrogels showed no dis-orderness as it is clear from its negative values (ΔS = -17.2, -461.16 and -16.42 kJ/mol for pAAc, 10%GG-g-pAAc and 20%GG-g-pAAc respectively).

Keywords: Gellan Gum; surface area analyzer; thermodynamics parameter; adsorption.

Sodium Alginate Grafted Hydrogel for Adsorption of Methylene Green and Use of the Waste as an Adsorbent for the Separation of Emulsified Oil

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Removal of noxious dyes and oils from the modern day industrial discharges is compulsory to safeguard humans, aquatic organisms and water quality and to prevent ecological damages induced by pollutants. The underscored problems were addressed by one pot fabrication of sodium alginate grafted poly (acrylic acid-*co*-N-vinyl formamide) [SA-g-p(AAc-co-VFA)] hydrogel. The hydrogel swelled in water up to 7665% due to water absorption through Fickian diffusion. The smart hydrogel efficiently performed sorption of methylene green (MG) from aqueous solution owing to outstanding swelling potential and electrostatic interactions. The maximum sorption potency of the adsorbent reached to 1915 mg g^{-1} with excellent removal at 5 and > 11 pH values. The MG-sorption followed pseudo second order kinetic and Langmuir isotherm models, thus indicating chemisorption of cationic-MG onto anionic sorbent due to the development of electrostatic bond. The used [SA-g-p(AAc-co-VFA)/MG] sorbent was tested for oil (toluene as oil probe) separation from its aqueous emulsion. The material exhibited 94% separation efficiency toward toluene eradication which remained unchanged for five successive runs. The remarkable swelling and sorption potencies of the hydrogel coupled with the outstanding toluene separation efficiency of the MG-sorbed hydrogel make the subject hydrogel a versatile material for relevant industrial and environmental applications.

Keywords: Hydrogel; Dye sorption; Oil separation; Environmental applications.

Essential elemental levels with Proton Pump Inhibitors in the biological samples of gastrointestinal disturbed patients residing in different cities of Sindh, Pakistan

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The prolonged bloating, abdominal discomfort, reflux, nausea, vomiting, diarrhea, stomach pain, and discomfort characterize a collection of digestive conditions known as gastric distress. Proton pump inhibitors (PPIs) remain the superior choice worldwide in antisecretory therapy in the evidence-based treatment of upper gastrointestinal disorders including gastroesophageal reflux disease, erosive esophagitis, dyspepsia and peptic ulcer disease. To digest the materials, a 2:1 ratio of HNO_3 (65%) and H_2O_2 (30%) has been employed in a microwave oven-assisted digestion process. Elemental concentrations were determined by flame atomic absorption spectrometry. The goal of this research was to evaluate the link between essential trace elements (zinc, iron, copper, calcium and magnesium) with proton pump inhibitors in samples of biological material, namely blood, serum, and urine of 350 gastrointestinal disturbance patients, who were inhabitants of different cities in Pakistan and ranged in age from 30-45 to 46 years. The biological specimens of reference subjects (n = 135) in the same age ranges have been analyzed for comparison analysis. The study concluded that most contributing factor was interaction of PPIs with essential and trace elements which disturbed the level of Zinc, Iron, Copper, Calcium and Magnesium, which produced different complications. The collected information will be useful in the treatment of gastrointestinal disturbed patients and enhance the chances of survival with better healthy life.

Keywords: Essential trace elements; Gastrointestinal disturbed patients; proton pump inhibitors; Flame atomic absorption spectrometry

Exploring Acyl Thiotriazinoindole Based Pharmacophores: Design, Synthesis, and SAR Studies with Molecular Docking and Biological Activity Profiling against Urease, *α*-amylase, *α*-glucosidase, Antimicrobial, and Antioxidant Targets

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A small library of acyl thiotriazinoindole (ATTI) based bioactive scaffolds was synthesized, instigated by taking the economical starting material Isatin, through a sequence of streps. The newly synthesized motifs were scrutinized for their potential to impede urease, *α*-glucosidase, DPPH, and *α*-amylase. Compound **5h** with para cyano group manifested the most pivotal biological activity among all, displaying IC_{50} values of 29.7 ± 0.8, 20.5 ± 0.5 and 36.8 ± 3.9 μM against urease, *α*-glucosidase, and DPPH assay, respectively. For α-amylase compound **5g** possessing a p-CH_3 at phenyl ring unfolded as most active, with IC_{50} value 90.3 ± 1.1 μM. Compound **5d** having bromo as substituent exhibited the most potent antibacterial activity, as well as highest potency against *Aspergillus fumigatus*. Derivatives **5b, 5e, 5i,** and **5j** also exhibited dual inhibition against both antibacterial and antifungal strains. The interaction pattern of derivatives clearly displayed their SAR, and their docking scores were correlated with their IC_{50} values. In molecular docking studies, the importance of interactions like hydrogen bonding was further asserted.

Keywords: Heterocycles: Acyl thiotriazinoindoles; Enzyme inhibition; Molecular docking; Antimicrobial.

Green-Mediated Synthesis of $NiCo_2O_4$ Nanostructures Using Radish White Peel Extract for the Sensitive and Selective Enzyme-Free Detection of Uric Acid

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The ability to measure uric acid (UA) non-enzymatically in human blood has been demonstrated through the use of a simple and efficient electrochemical method. A phytochemical extract from radish white peel extract improved the electrocatalytic performance of nickel-cobalt bimetallic oxide (NiCo2O4) during a hydrothermal process through abundant surface holes of oxides, an alteration of morphology, an excellent crystal quality, and increased Co(III) and Ni(II) chemical states. The surface structure, morphology, crystalline quality, and chemical composition were determined using a variety of analytical techniques, including powder X-ray diffraction (XRD), scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HR-TEM), and X-ray photoelectron spectroscopy (XPS). The electrochemical characterization by CV revealed a linear range of UA from 0.1 mM to 8 mM, with a detection limit of 0.005 mM and a limit of quantification (LOQ) of 0.008 mM. A study of the sensitivity of NiCo2O4 nanostructures modified on the surface to UA detection with amperometry has revealed a linear range from 0.1 mM to 4 mM for detection. High stability, repeatability, and selectivity were associated with the enhanced electrochemical performance of non-enzymatic UA sensing. A significant contribution to the full outperforming sensing characterization can be attributed to the tailoring of surface properties of NiCo2O4 nanostructures. EIS analysis revealed a low charge-transfer resistance of 114,970 Ohms that offered NiCo2O4 nanostructures prepared with 5 mL of radish white peel extract, confirming an enhanced performance of the presented non-enzymatic UA sensor. As well as testing the practicality of the UA sensor, blood samples from human beings were also tested for UA. Due to its high sensitivity, stability, selectivity, repeatability, and simplicity, the developed non-enzymatic UA sensor is ideal for monitoring UA for a wide range of concentrations in biological matrixes.

Keywords: non-enzymatic uric acid sensor; phytochemicals; radish white peel extract; biological matrix.

Polyphenols: Isolation, Purification, Characterization and Evaluation of Biological Activities

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The purpose of this study was to explore the cardioprotective and anti-inflammatory effects of polyphenol-rich extracts from cucurbitaceae family members, including Cucurbita pepo, C. moschata, and C. maxima, on rat models. The initial crude extracts from these cucurbits were further separated into hexane, chloroform, ethyl acetate, butanol, and aqueous ethanol fractions, labeled as HEF, CHF, EAF, BUF, and AEF, respectively. Of these, AEF yielded the highest amount, followed by BUF, HEF, EAF, and CHF in descending order. Notably, EAF contained the greatest concentration of total phenolics, flavonoids, and flavonols. In terms of antioxidant activity, EAF demonstrated the most potent DPPH radical scavenging capability, succeeded by CHF, BUF, AEF, and HEF. EAF also exhibited the strongest reducing potential among the fractions. RP-HPLC analysis identified various phenolic acids and flavonoids across the cucurbita fractions, including ferulic acid, vanillic acid, p-coumeric acid, gallic acid, p-hydroxybenzoic acid, chlorogenic acid, catechin, rutin, quercetin, myricetin, and kaempferol. Doses of 250 and 500 mg/kg body weight of cucurbita fractions were administered orally to male WKY rats daily for 21 days. The rats' body weight, heart rate, and blood pressure were monitored bi-weekly. Oxidative status assessments were conducted using plasma samples to measure levels of malondialdehyde (MDA), superoxide dismutase (SOD), reduced glutathione (GSH), nitric oxide (NO), and total antioxidant capacity (TAC). At the study's conclusion, surgical assessments including blood pressure, pulse wave velocity (PWV), and echocardiograms (ECG) were performed. The findings indicated that EAF from cucurbita significantly enhanced antihypertensive and antioxidant activities in the SHR rat group.

Keywords: Quercetin; Ferulic acid; gradient elusion; pulse wave velocity; SHR

Synthesis and characterization of biologically active flurbiprofen amide derivatives as selective prostaglandin-endoperoxide synthase II inhibitors: *In vivo* anti-inflammatory activity and molecular docking

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A novel series of twenty two flurbiprofen amides **(1-22)** were designed and synthesized in good to excellent yields by reacting flurbiprofen acid with various aromatic/aliphatic primary amines in the presence of 1,1-carbonyldiimidazole (CDI) in basic medium using acetonitrile as solvent. Structures of the synthesized derivatives were elucidated with the help of HR-ESI-MS, ^{1}H-, and ^{13}C NMR spectroscopy and finally screened them for their *in-vivo* anti-inflammatory potential using carrageenan induced mice paw oedema assay. Among the series, four compounds **(8, 14, 15,** and **20)** displayed excellent activity ranging from 59.0 to 77.7 % decrease, while eight compounds **(1, 3, 7, 10, 12, 13, 17,** and **18)** exhibited good activity in the decrease range of 37.0-50.0 %. Additionally, four compounds **(2, 6, 16,** and **22)** attributed less activity, while the remaining six compounds **(4, 5, 9, 11, 19,** and **21)** were found to be inactive. Furthermore, the *in-silico* studies were executed on the synthesized derivatives in order to explain the binding interface of compounds with the active sites of prostaglandin endoperoxide-synthase II enzyme.

Keywords: Flurbiprofen; amides; anti-inflammatory; Molecular Docking

Structure-Based Design and Synthesis of Trolox-1,3,4-Oxadiazole Hybrids with Potential Multi-Target Bioactivities

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We have focused our research on the synthesis of oxadiazole-based Trolox derivatives following multi-step reaction and assessment of their anticholinesterase inhibitory activities. Trolox was esterified with ethanol in the presence of a catalytic amount of sulfuric acid and further subsequent substitution with hydrazine hydrate yielded the acyl hydrazide. The acyl hydrazide upon condensation with various substituted aldehydes resulted in the corresponding Schiff's bases. The cyclization of Schiff's bases was carried out in iodine to obtain the target oxadiazoles of Trolox. The structures of the synthesized compounds were confirmed via UV, ^{1}HNMR, and Mass spectroscopic techniques. The studies of bioactivities both *in silico* and *in vitro* for the synthesized compounds reflect that they can act as leads for the design and synthesis of drugs.

Synthesis and Characterization of Iron Oxide (II, III), its Drug Conjugates with Thalidomide, and their Biological Applications

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Thalidomide, known for its antiangiogenic, anti-inflammatory, immunomodulatory, hyposedative, and antiemetic properties, is hindered by its teratogenic effects. This study aims to enhance its therapeutic potential through conjugation with iron oxide nanoparticles (FeO-NPs). FeO-NPs were synthesized via the coprecipitation method employing ferric chloride and ferrous sulfate as precursors. Thalidomide was successfully conjugated with FeO-NPs, as evidenced by UV-Vis spectroscopy, FTIR, EDX and XRD analysis. UV-Vis spectroscopy revealed absorption peaks at 218 nm for FeO-NPs, 291 nm for thalidomide, and between 200–300 nm for the conjugates, indicating successful conjugation. FTIR analysis exhibited characteristic Fe-O stretching vibrations, affirming the formation of FeO-NPs and the presence of thalidomide within the conjugates. In the XRD analysis, the disappearance of thalidomide's characteristic peaks further confirmed its successful loading onto FeO-NPs. EDX further validated the composition, showing prominent peaks for iron (Fe), oxygen (O), and carbon (C), signifying a pure composite structure devoid of impurities. Together, these findings confirm the effective synthesis and characterization of the FeO-thalidomide conjugates. Anticancer activity and inhibition of phospholipase A2 (PLA2) were evaluated for various doses of thalidomide and its derivatives. Among them, FT4 exhibited the highest PLA2 inhibition at 71%, followed by FT3 (67%), FT2 (44%), and FT1 (11%). EDTA demonstrated potent inhibition at 90%, highlighting the dose-dependent nature of inhibition and the potential of AS4 for anti-PLA2 therapy. These findings underscore the potential of thalidomide derivatives, particularly FT4, in enhancing anticancer activity and inhibiting PLA2 at relatively low concentrations. The observed results warrant further mechanistic exploration for therapeutic insights. Conjugation with FeO-NPs enhances the therapeutic potential of thalidomide by improving its efficacy as an anticancer agent and inhibitor of PLA2. Further research into the mechanistic aspects of these conjugates is warranted to elucidate their full therapeutic potential.

Keywords: Drug delivery; Nanoparticles; Pharmaceuticals; Inflammatory mediators.

DNA Comet Assay for Screening of Un-irradiated and Irradiated Samples of Beans, Pulses, Tree nuts, Spices and Meats

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Food irradiation has many applications like preservation of different kinds of foods, reduction of pathogenic and spoilage microorganisms to enhance the hygienic quality of foods. The technology is in use for several kinds of foods throughout the world. For proper surveillance on the use of the technology reliable screening methods for irradiated foods are needed and for this purpose DNA comet assay has been investigated for different kinds of foods containing DNA material. The long molecules of DNAs are highly susceptible to radiation (electron beam, X-rays or γ - rays). The irradiation may cause single or double strand breaks of DNAs in irradiated foods but no damage in controlled samples of food. This damage of DNAs serves as the marker for differentiating irradiated and un-irradiated foods. The method was performed using irradiated and controlled samples of beans, pulses, tree nuts, spices and meat. They were irradiated to different permissible radiation doses (0.5 - 20 kGy) with help of electron beam linear accelerator (Germany). The isolation and fixing of DNAs on microscope slides, lysis of DNAs and then electrophoresis of DNAs was performed and then silver staining was done for observations of DNAs under microscope. The stains in the oval/round shapes indicate un-irradiated (controlled) and stains in different shapes of comets with tails towards anode indicated the irradiated samples. These experiments led to the conclusion that screening of irradiated and un-irradiated food samples was possible and the method was useful for surveillance of the food irradiation technology.

Keywords: Plant and animal Foods; Irradiation of Foods; DNA Comet assay; Screening of un-irradiated and irradiated food samples

Increasing Use of Plastic Bottle Beverages in Pakistan: A Potent Source of Endocrine Disruptor Phthalates

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Phthalates (PAEs) are widely used as plasticizers in the production of polyvinyl chloride and polyethylene terephthalate plastics. However, due to their extensive use, phthalate esters are considered ubiquitous environmental concerns. PAEs can contaminate beverages and packaged food while they are being packed, transported, and stored. PAEs are endocrine-disrupting compounds (EDCs) that can have serious consequences on human health. The purpose of this study was to measure the amount of phthalate esters that leached from beverages kept in plastic bottles such as mineral water, carbonated drinks and fruit juices commonly consumed among local population. In addition, plastic bottles were characterized by FTIR, which confirms the presence of PAEs by evaluating the aromatic esters and C-H wagging peaks at 1713 cm $^{-1}$ and 722 cm $^{-1}$ respectively. Furthermore, DSC analysis of plastic bottles revealed distinct Tg and Tm values for bottles that are amorphous in nature. All of the fruit juices and carbonated liquids were acidic, with pH levels ranging from 2.25 to 3.73. According to chromatographic analyses, total of 10 PAEs were leached and identified from mineral water bottles. Among them, dimethyl phthalate, bis(2-methoxyethyl) phthalate, diethyl phthalate, and dibutyl phthalate were the major leached PAEs found in the range 9–112.50 μg L−1. In addition, mixed fruit juices had the most PAEs leaching (71.93g/L), followed by strawberry juices (31.35 g/L), citrus fruit juices (20.64 g/L), and fleshy fruit juices (18.61g/L). Different PAEs such as DPrP, DiBP, DPeP, DCHP, BBzP, DEHP, and DOP were validated by GC-MS. Estimated daily intakes (EDIs) of the PAEs from fruit juices ranged from 0.087 to 0.543 μg/kg/bw. Non-carcinogenic risks concerning PAEs in juices were found to be within safe levels (less than one). DEHP in fruit juices exhibited the potential carcinogenic effects on humans. Overall studies indicate that carbonated drinks and juice packed in plastic bottles are more prone to phthalate leaching owing to acidic pH and high temperature exposure in our Country, therefore phthalate should be replaced with other plasticizers.

Keywords: Phthalate esters; plastic bottles; endocrine disruptors; beverages

Doping Superalkalis on Chlorine Substituted Coronene: Interactive Design Computation of New NLO Materials for Optoelectronics

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The significant applications of nonlinear optical (NLO) materials in modern technology have stimulated considerable interest in their fabrication. Ongoing efforts are being made to develop materials that exhibit a substantial nonlinear optical response. To this end, the current study explores theoretically designed complexes (I-XIII) of chlorine-substituted coronene doped with superalkalis (Li3S, Li3O, and Li3N) using density functional theory (DFT). The HOMO-LUMO energy gap (*Eg)* is significantly narrowed by superalkali doping. The energy gap of designed complexes of C24Cl6H6 is reduced up to 0.72 eV. Furthermore, this strategy led to a significant increase in the hyperpolarizability values, with the maximum first hyperpolarizability (*βo*) value found to be 8.4 ×104 au. The TDOS and PDOS spectral analyses are used to explore the contribution of different segments in frontier molecular orbitals. NCI analysis is performed to better understand the interaction between superalkali and C24Cl6H6 substrate molecule. TD-DFT calculations are also carried out for UV-Vis analysis and crucial transition states of newly designed structures. All the obtained computational results revealed that superalkali-doped C24Cl6H6 complexes are thermodynamically stable NLO materials with enhanced NLO responses. Hence, these materials are recommended for the construction of advanced NLO applications.

Keywords: Chlorine substituted coronene (C24Cl6H6), Superalkali (Li3S, Li3O, and Li3N) doping
Nonlinear optical response (NLO), Density functional theory (DFT)).

Heavy metal pollution in the urban-rural interfaces: A threat to human health and ecosystem sustainability

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Heavy metal contamination in urban-rural interfaces poses a significant threat to human health and biodiversity, necessitating further research to understand the anthropogenic sources, ecotoxicity, and contamination mitigation. The purpose of this research was to examine the levels of heavy metals in vegetables grown in urban-rural interfaces and the effects these metals may have on human health. Eight heavy metals, including cobalt (Co), nickel (Ni), manganese (Mn), iron (Fe), chromium (Cr), lead (Pb), cadmium (Cd), and zinc (Zn), were tested in wastewater, soil, and vegetable samples obtained from three sectors (DS1, DS2, and DS3). Heavy metal transfer factors were determined and displayed for three different vegetables (spinach, tomatoes, and cabbage) across three different sectors. The results demonstrated that the transfer factors varied for each metal, depending on the sector and vegetable. Although the levels of heavy metals in the wastewater, soil, and vegetables were found to be within acceptable limits, the results demonstrated that cadmium and lead presented serious health hazards to children and adults alike. A modest health risk was found as a result of the intake of these metals, according to the analysis of daily intake of heavy metals (DIM) values for both adults and children across three sectors. The data indicate that cadmium and lead pose considerable health concerns to both adults and children. There was a strong relationship between the Cr concentration in wastewater of sector DS1 and sector DS2, indicating that Cr concentrations are affected by comparable geological factors in both sectors. The study suggests that heavy metal levels in soil, wastewater, and vegetables should be monitored regularly and contamination in agricultural contexts must be managed to protect public health.

Keywords: Heavy metal; Anthropogenic; Contamination; Health risk; Transfer factors; Daily intake

Synthesis of Sodium Alginate – Kernel Powder Blend Beads and their Surface Properties in Removal of Heavy Metals from Aqueous Media

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The present work focuses on synthesis of sodium alginate, kernel powder beads separately and their mixed blend beads. Characterization conducted by using scanning electron microscopy (SEM), particle size, FTIR spectroscopy and X-ray diffractometry (XRD). Point of zero charge (PZC) of these three adsorbents studied by using $NaNO_3$ as appropriate background electrolyte. Batch adsorption technique conducted for removal of heavy metals (Pb, Cu and Ni ions) in aqueous media. The applicability of Langmuir and Freundlich models is tested to determine the mechanism of sorption reaction. The heat of adsorption of these models are also compared. The thermodynamic parameters indicate that heavy metals removal is entropy driven ion exchange mechanism.

Keywords: Adsorption, Characterization, PZC, Ion Exchange

Microwave Plasma: An Innovative Strategy for Enhancing Structural and Photocatalytic Properties of Silver Zirconate/GO Nanocomposite

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Microwave plasma generated at low pressure has garnered significant attention as a highly effective method for enhancing the opto-physical attributes of materials. In this work, silver zirconate graphene oxide (Ag2Zr4/GO) nanocomposite was synthesized by hydrothermal route and then exposed to microwave oxygen plasma to enhance the opto-physical attributes for photocatalytic degradation of Basic Fuchsin (BF) dye. The physico-chemical characteristics of materials were analyzed employing both conventional and advanced analytical techniques. XRD showed that plasma-treated Ag2Zr4/GO nanocomposite retained crystallite size of 80 nm with a tetragonal crystalline structure. SEM-EDX indicated high surface porosity of plasma-treated Ag2Zr4/GO nanocomposite and an average particle size of 220 nm. FTIR confirmed the successful integration of Ag2Zr4 nanospheres with GO. UV–vis spectroscopy showed characteristic absorption bands for photocatalysts in the range of 400–530 nm. DLS provided a z-average of 230 ± 5 nm and a zeta potential of −14.01 ± 2 mV for plasma-treated Ag2Zr4/GO nanocomposite. The photodegradation study showed 99 % degradation of BF in 45 min and significant antibacterial activity against *E. coli* and *S. aureus* strains by plasma-treated Ag2Zr4/GO nanocomposite. A reusability study demonstrated that the catalysts maintained effectiveness over five consecutive cycles. Kinetic analysis showed the experimental data aligned well with the Behnajady-Modirshahla-Ghanbery (BMG) model. These findings suggest that plasma-treated Ag2Zr4/GO nanocomposite is a promising candidate for organic pollutant oxidation in environmental remediation applications.

Keywords: Photocatalysis, Basic Fuchsin, Sunlight illumination, Behnajady-Modirshahla-Ghanbery, Microwave plasma

A Photo-responsive Sn and Pt doped Zirconia Catalyst for the degradation of Acid Yellow-76

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Monoclinic zirconia (ZrO_2) and Sn/Pt doped or co-doped zirconia (Pt@ZrO_2, Sn@ZrO_2, Sn/Pt@ZrO_2) were produced through microwave-assisted protocol. The synthesized materials were characterized and tested for their ability to degrade Acid Yellow 76 (AY-76) under UV (blue) and visible (green) light. SEM images showed that zirconia particles had a smooth morphology with 80-85 nm in size. In contrast, ultra-small Sn and Pt particles were found scattered on the surface of zirconia. The low surface area (48m^2/g) of Sn/Pt@ZrO_2 than pure ZrO_2 (61m^2/g) attributed to the surface pore blockage by ultra-small size nanoparticles (NPs) of Sn and Pt. Fluctuation in the rate of photo-degradation of AY-76 with different reaction parameters was investigated. The results indicated that, under optimal reaction conditions; substrate solution (10mL), concentration (10ppm), catalyst (0.15g), pH (6-8), oxidant (H_2O_2: 2mL), stirring (1200rpm), time (90min) and temperature 60^{0}C, Sn/Pt@ZrO_2 demonstrated excellent photocatalytic activity towards AY-76 degradation. Furthermore, Density Functional Theory (DFT) and experiments confirmed the role of the dopant (Sn and Pt) on the transformation of ZrO_2 towards photo-responsive region. Overall, the findings provide insight into the potential use of these catalysts as a more potent alternative for prevailing wastewater treatment processes.

Keywords: Acid Yellow, Sn/Pt@ZrO_2, Photodegradation

A simple 2,4-dihydroxyacetophenone based fluorescent chemosensor for detection of copper(II) ion

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The detection of copper ions is of significant importance due to their widespread use and potential toxicity at elevated concentrations. In this study, a bis Schiff's base compound; 4-(1-(cyclohexylidenehydrazono) ethyl) benzene-1,3-diol (**BS**) was used for the first time based on "Turn off" fluorescent chemosensing of Cu(II) ion in water samples with characteristics of aggregation induced enhanced emission (AIEE) at 500 nm upon excitation at 405 nm. **BS** showed high selectivity towards Cu(II) ions which displayed considerable fluorescence quenching and was found negligible inference effect by other metal ions in mixed solution of methanol-water (v/v,1:9) at pH 8. Fluorescence intensity of **BS** was observed to decrease due the formation of non-fluorescent complex (**BS@Cu**) which could be associated to the paramagnetic effect caused by spin-orbit coupling of Cu (II). The stoichiometric ratio of BS with Cu (II) was determined to be 1:1 using Job's method. DFT simulations was performed to gain theoretical insight into the interaction of Cu(II) with **BS**. The value calculated for limit of detection (LOD) was 0.26μM, allowing the identification of trace amounts of the analyte in complex environmental matrices. Significant recovery of above 95% was achieved from spiked water samples. This novel turn-off fluorescent sensor offers a simple, cost-effective, and reliable method for the rapid detection of copper ions, making it a valuable tool for environmental monitoring and ensuring the safety of water resources.

Keywords: Chemosensor, Environmental monitoring, Fluorescence quenching, Heavy metal, Trace analysis

Synthesis and Computational Study of an Optical Fluorescent Sensor for Selective Detection of Ni^{2+} Ions

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The presence of an abnormal amount of Ni^{2+} in the human body causes various health issues. Therefore, this work aimed to synthesize the curcumin-based fluorescence-on sensor **P** [2,6-bis((E)-4-chlorobenzylidene)-cyclohexan-1-one] that was capable of selectively responding to Ni^{2+} ions in aqueous solution. The structure of **P** was confirmed by ^{1}H NMR and Fourier transform infrared (FTIR) spectroscopy. The Ni^{2+} ion sensing was based on the fluorescence enhancement of the fluorophore (**P**) in neutral aqueous medium. The response of the **P**-based sensor was highly selective toward Ni^{2+} ions, whereas the possible interferences from other metal cations were negligible. **P** had a fast response; it was selective and had a sensitive detection limit (LOD = 2×10^{-10} M) toward Ni^{2+} ions in neutral medium with a high association constant (K) value of 3.6×10^{5} M^{-2} for the complex formation between the **P** and Ni^{2+} ions. Job's plot and DFT calculations proved that the binding stoichiometry of **P** for Ni^{2+} was 2:1. **P** was recovered using EDTA as a chelating agent after being employed as a fluorescent sensor. These characteristics ensured the potential use of **P** as a new class of chemosensor for environmental applications.

Keywords: Fluorescent-on; Chemoensor; Ni^{2+} ion; limit of detection

Green Synthesis of Mono and Bimetallic Nanoparticles and their Applications

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In this study, we report the green synthesis of MgO@biochar using *Ziziphus mauritiana*, *Prosopis juliflora*, and *Azadirachta indica* as eco-friendly sources. The synthesized MgO@biochar-Zm, MgO@biochar-PJ, MgO@biochar-AI was thoroughly characterized using various analytical techniques including Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), UV-visible spectroscopy, and zeta sizer analysis. These characterizations confirmed the functional composition, porous texture, and highly crystalline cubic structure of the MgO@biochar-ZM, MgO@biochar-PJ, MgO@biochar-AI nanocomposite with particle size of 91.28, 78.8 and 43.8 nm. The MgO@biochar-Zm, MgO@biochar-PJ and MgO@biochar-AI demonstrated significant potential as a photocatalyst for the degradation of Eosin Y (EY) dye. Under optimized conditions—90 minutes of reaction time, 50, 60 and 80µL of catalyst dose, 20 ppm dye concentration, and ambient room temperature the MgO@biochar-Zm, MgO@biochar-PJ, MgO@biochar-AI achieved 97%, 95% and 94 degradation of EY dye in an aqueous solution. The study also highlighted the excellent reusability of the MgO@biochar-Zm, MgO@biochar-PJ and MgO@biochar-AI retaining their catalytic efficiency up to the fifth cycle of use, which underscores the durability and effectiveness of the catalyst. Furthermore, the application of MgO@biochar-Zm, MgO@biochar-PJ and MgO@biochar-AI for the degradation of EY dye was extended to real samples, showcasing its practical applicability in environmental remediation. The findings of this research suggest that MgO@ biochar-ZM, MgO@ biochar-PJ, MgO@ biochar-AI are promising and sustainable photocatalyst for the treatment of dye-contaminated wastewater, contributing to the development of green chemistry and sustainable environmental practices.

Adsorptive Removal of Cetyltrimethyl Ammonium Bromide (CTAB) Surfactant from Aqueous Solution: Crossbreed Pilot Plant Membrane Studies

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Magnetic carbon nanocomposite (MCNC) was prepared from peanut shells and then characterized by FTIR, SEM, TGA/DTA and BET surface area. The removal of cetyltrimethyl ammonium bromide (CTAB) surfactant from aqueous solution was carried out by MCNC and membrane. The effect of contact time, initial concentration of CTAB and the temperature on the adsorption of CTAB was also investigated. Initially, the adsorption of CTAB on MCNC was rapid up to 20 min and then gradually slowed down. Different kinetic models i.e. 2nd pseudo order kinetics, power function and intraparticle diffusion were applied to determine different kinetic parameters. Intraparticle diffusion model showed that the adsorption of CTAB is a diffusion controlled process. Thermodynamic parameters i.e. ΔH° (-33.74 kJ/mol), ΔS° (0.98 J/mol K) and ΔG° (-62.91 kJ/mol, −64.37 kJ/mol and −66.33 kJ/mol) were calculated and the process was found to be exothermic and spontaneous in nature. The prepared adsorbent (MCNC) was used for controlling fouling of ultrafiltration (UF), nanofiltration (NF) and reverse osmosis (RO) membranes caused by CTAB. Improved permeate fluxes and percent retention of CTAB were observed for MCNC crossbreed membrane. About 100% retention with no effect on permeate flux was observed with RO membrane when MCNC pretreatment was applied.

Keywords: Nanocomposite, Membrane, Adsorption, Thermodynamic.

Water Quality Profile of North Eastern Pakistan

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Water is essential for human survival, yet the rapid increase in global population and the associated human activities have led to a swift and troubling decline in both the quantity and quality of freshwater supplies. Across the world, water-stressed regions are expanding rapidly due to unsustainable water usage, excessive extraction beyond natural recharge rates, and significant changes in rainfall patterns. This growing water shortage is affecting billions of people, creating economic difficulties and lowering the quality of life. At the same time, freshwater quality has been severely impacted by careless, unregulated, and environmentally damaging practices. The responsibility for this environmental crisis rests solely with humans. As a result, we are seeing a rise in public health issues and lasting damage to aquatic ecosystems. There is an urgent need to address the issues of water quantity and quality on both global and regional scales, especially in Pakistan. Right intervention is required to safeguard the existing water resources. In addition to this, excess water from seasonal floods could become a valuable resource if we build the right infrastructure to store and preserve it. Our recent research into water quality in northeastern Pakistan shows a worsening situation in both the amount and quality of freshwater. Bacterial contamination is widespread, and in some cases, elevated levels of heavy metals and anions have been detected, posing a serious risk to the region's freshwater supply.

Keywords: Water, Fresh water, Contamination, Health Risks

Hepatoprotective Potential of *Vitis vinifera* Silver Nanoparticles against Acrylamide Induced Liver Damage in Rabbits

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The *Vitis vinifera* (black grapes) used as traditional medicine owing to its immense pharmacological properties. The foremost downside of herbal-based drugs is their poor bioavailability, to trounce this we synthesized herbal based silver nanodrug using aqueous extract of *Vitis vinifera* and accessed its effect against acrylamide induced hepatotoxicity in rabbits. The green synthesized reduced silver-Nanoparticles (Ag-Nanoparticles) were characterized using Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction analysis (XRD), scanning electron microscopy (SEM) and Liquid Chromatography mass spectrometry (LCMS-MS) analysis. After acclimation period, biochemically tested healthy trial animals were divided into seven groups (n=3) and differentiated by ear tagging. Experimental animals were injected with acrylamide (50mg/ml per kg BW) for 6 days and then orally treated with aqueous extract of *Vitis vinifera* and synthesized AgNPs at three dose concentrations (50, 100, and 150mg/ml) for 20 days. Serum levels of hepatic markers (Alanine aminotransferase (ALT), Aspartate aminotransferase (AST), and (ALP)) and oxidative stress indicators (CAT (Catalase), SOD (Superoxide dismutase), and GPx (glutathione peroxidase)) were accessed. Results from Mass spectral analysis revealed that Resveratrol, trans-ϵ-Viniferin were the major hepatoprotective phenolic compounds. Analytical observations confirmed the stabilization and spherical shape of green synthesized Ag-Nanoparticles with an average size of 20.09nm. Further results indicate that treatment with aqueous extract of *Vitis vinifera* and synthesized AgNPs attenuated acrylamide induced hepatotoxicity in a dose dependent manner as demonstrated by the significant ($p<0.05$) decrease in the levels of ALP (45.2 ± 1.7 UL), ALT (37.4 ± 1.2 UL), and AST (30.7 ± 0.9 UL) on highest dose concentration of synthesized AgNPs (150 mg/ml) as compared to Acrylamide group. This was also evidenced by significant ($p<0.05$) increase in the levels of oxidative stress markers i.e. CAT (930.7 ± 2.3 IU/mL), SOD (6.7 ± 0.02 IU/mL), and GPx (4.0 ± 0.01 IU/mL) in blood on the same dose concentration of synthesized AgNPs as compared to Acrylamide group. Our results concludes that synthesized AgNPs using aqueous extract of *Vitis vinifera* have protective effect against acrylamide hepatocellular oxidative stress.

Keywords: Hepatotoxicity; *Vitis vinifera* aqueous extract; synthesized AgNPs; hepatoprotective potential

Phenolic Profile of Seedless *Ziziphus mauritiana* Fruits and Leaves Extracts *with In Vivo* Antioxidant and Anti-inflammatory Activities: Influence on Pro-Inflammatory Mediators

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The present study aimed to assess the antioxidant and anti-inflammatory activities of polyphenol-rich extracts of seedless variety of *Ziziphus mauritiana* (SZM). Reverse Phase High Performance Liquid Chromatography (RP-HPLC) analysis of SZM leaves and fruit extracts in ethanol revealed the presence of sixteen phenolics including chlorogenic acid, *p*-coumeric acid, gallic acid, kaempferol, rutin and quercetin. Leaf extract showed higher total phenolic and total flavonoid contents (177.6 mg/100 g and 46.2 mg/100 g) than in fruit extract (137.8 mg/100 g and 14.1 mg/100 g). The leaf extract exhibited higher DPPH radical-scavenging activity (63.5%) than the fruit extract (58.2%). The anti-inflammatory activity was evaluated on carrageenan-induced rat model and suppression of inflammatory biomarkers was studied. The fruit extract exhibited remarkable inhibition (98.1%) at the dose level of 500 mg/kg body weight (BW), comparable to the standard drug indomethacin (98.4%). Both extracts suppressed the inflammatory biomarkers and more pronounced results showed by the fruit extract including C-reactive protein, interleukin, tumour necrosis factor. The leaf extract demonstrated the higher antioxidant potential as evident from the superoxide dismutase, catalase, malondialdehyde, glutathione peroxidase and glutathione levels. These findings suggest that SZM leaf and fruit extracts possess potential antioxidant and remarkable anti-inflammatory properties and can play a significant role in mitigating oxidative stress.

Keywords: HPLC analysis; Polyphenols; Inflammation; Oxidative stress

Bioactive profile of *Ocimum americanium* Antimicrobial, Antibiofilm and Antipellicule Assays

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The assessment of phytochemical constituents and biological activities of plant extracts is paramount for discovering effective medicines. In this study *Ocimum americanum*, a medicinal plant from the Lamiaceae family, and extracted its leaves using 80% methyl alcohol, *n*-hexane, chloroform and ethyl acetate fractions. Qualitative phytochemical screening confirmed the presence of proteins, tannins, alkaloids, saponins, carbohydrates and flavonoids. Antibacterial, antibiofilm and antipellicle activities were systematically evaluated against *Clavibacter michiganensis subsp. michiganensis*, *Erwinia Carotovora*, *Enterobacterial common antigen*, *Klebsiella Pneumoniae* and *Xanthomonas Vesicatoria*. Antibacterial activity of *Ocimum americanum* and their fractions methyl alcohol and chloroform extracts exhibited prominent antibacterial efficacy. At the concentration of 10, 15,20 and30 µg/ml. Against *Clavibacter michiganensis subsp. michiganensis* methyl alcohol extract showed the highest zone of inhibition (19.00±1.00 mm), while against *Erwinia Carotovora*, methyl alchol and chloroform extracts displayed strong inhibitory effects. For *Enterobacterial common antigen* ECA, methyl alcohol and *n*-hexane extracts exhibited significant inhibition. Regarding antibiofilm activity, ethyl acetate extracts at concentrations of 15 µg/ml and 20 µg/ml consistently reduced biofilm formation in *Xanthomonas Vesicatoria* , *Enterobacterial common antigen*, and *Erwinia Carotovora* strains. Notably, the methyl acetate extract at 10 µg/ml exhibited promising results, inhibiting bacterial growth for ECA, ECC, and KP strains. For antipellicle activity, all extracts, including methyl alcohol, *n*-hexane chloroform, methyl alcohol, and *n*-hexane, showed strong inhibition against the bacterial strain Klebsiella Pneumoniae (KP). These findings underscore the potential of specific combinations of *Ocimum americanum* extracts in reducing bacterial growth, biofilm formation and pellicle layer formation. This research offers valuable insights for the development of antibacterial agents and biofilm inhibition strategies, emphasizing the significance of natural compounds in medicinal application.

Determination of Phytochemical Constituents of Choro (*Angelica glauca*) Leaves Extracts and their Biological Studies

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In this study, the leaves of Choro (*Angelica glauca*) were evaluated for occurrence of antioxidant components and valuable nutrients which are distributed wildly in hilly areas of Pakistan especially in Azad Kashmir. Extraction of leaves was carried out by maceration using solvents of various polarity such as *n*-Hexane, Chloroform, Ethyl acetate, *n*-Butanol, and Methanol. Qualitative and quantitative analysis was conducted for phytochemicals such as flavonoids, alkaloids, steroids, tannins and saponins. The flavonoid and phenolic contents were examined by using spectrophotometric techniques. The Choro *Angelica glauca* leaves showed that the *n*- Butanol shows higher concentration in total flavonoid contents (TFC) i.e. 80.87mg/100g and *n*-Hexane shows lower concentration i.e. 10.57 mg/100g CE. In total phenolic contents (TPC) tests showed that methanol contains a higher concentration i.e. 676.71 mg/100g GAE and *n*- Hexane shows lower concentration i.e.103.26 mg/100g GAE. The 2, 2-Diphenyl-1-picrylhydrazyl (DPPH) scavenging action was carried out. Antioxidant potential was measured by DPPH free radical having higher value for methanol i.e. 85.60% and lower for chloroform i.e. 38.18%. Similarly, the reducing power of methanolic extract was also measured. Triton X-100 a synthetic compound was used a positive control that give maximum percentage lysis value 100.01% so hemolytic activity of *Angelica glauca* leaves extract was evaluated and maximum percentage lysis was obtained for *n*-Hexane extracts i.e. 8.71% and methanol shows lowest concentration i.e. 0.31%. The thrombolytic activity of *Angelica glauca leaf* extracts was evaluated against human red blood cells, and the maximum percentage of clot lysis was 59.10% in chloroform extract, it was concluded from the research and results shows that all the extracts of Choro *Angelica glauca* leaves showed considerable pharmacological properties and also exhibited good antioxidant, antimicrobial and less cytotoxicity activity. Overall, the presented results reveal that Choro (*Angelica glauca*) extract is capable of being employed in nutra-pharmaceutical industry.

Keywords: *Angelica glauca*, antioxidant, antimicrobial, bioactive compound

Computational modeling of proton pump inhibitors against 4F5S, 1IK3, and 3TOP targets: a study on advanced glycation end products

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The study analyzed the computational validation of various drugs against transcription regulator genes, including 1IK3, 4F5S, and 3TOP. Antiviral drugs like Acyclovir, ribavirin, and sobosofovir were tested. Sobosofovir showed the highest free binding energy (-8.5 ΔG (kJ mol−1) against 1IK3. Antihypertensive drugs like Carvedilol, Atorvastatin, Rousovastatin, and Atenolol were used. Rousovastatin showed the highest free binding energy (-8.1 ΔG (kJ mol−1) against 1IK3. Proton pump inhibitors like Famotidine, Esomeprazole, Pentoprazole, Dexlonsprazole, Lansoprazole, Omeprazole, and Rabeprazole were tested against 1IK3, 3TOP, and 4F5S. Lansoprazole had the highest free binding energy (-8.7 ΔG (kJ mol−1) against 1IK3. The study analyzed compounds for potential α-glucosidase inhibitory potential. None of the antiviral drugs showed any inhibition of α-glucosidase, while Acyclovir and ribavirin showed mild antioxidant activity in the DPPH assay. However, Acyclovir and Ribavirin showed slightly variable results in H2O2 assay. Antihypertensive drugs did not inhibit α-glucosidase, but moderate antioxidant activity was recorded in Atorvastatin, rousovastatin, and atenolol. PPI showed significant inhibition in some compounds. Omerprazole showed significant inhibition of α-glucosidase, followed by Famotidin and Pentoprazole. All other drugs were found inactive. The study analyzed compounds with significant antidiabetic potential for potential antiglycation inhibitory potential. The highest inhibition of AGES in nonoxidative mode was recorded in Omeprazole (IC50 1.12 mg/mL), followed by pentoprazole (IC50 1.56 mg/mL). Omeprazole showed a protective effect compared to the control, while moderate protective effects were observed in esomeprazole. The anti-inflammatory activity of all samples was analyzed using a 15-Lox assay, with none of the antiviral drugs showing any activity. Atorvastatin showed slight inhibition of 15-Lox, while esomeprazole, omeprazole, and lansoprazole were the most effective. Overall, the study highlights the potential of repurposing medications like omeprazole and esomeprazole in managing inflammation and diabetes.

Keywords: Repurposing of drugs: Stability study: Proton pump inhibitors: Interaction analysis: Bioavailability score: Molecular docking

Synthesis and Pharmacological Screening of Thiourea Derivatives

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Synthesis of thiourea derivatives by the condensation of phenyl isothiocyanate with various substituted aromatic amines in dry acetone has been reported. All the thiourea derivatives were further confirmed from melting point, 1HNMR spectrum and elemental analysis. The compounds are screened for anti-bacterial activity against bacteria *Agrobacterium tumefacien*, *Staphylococcus aureus* and *Proteus vugaris* using agar well diffusion method.

Hydrothermal Synthesis of Quaternary FeBiZn Selenide Nanocomposites for Efficient Degradation of Organic Contaminants in Aqueous Solutions

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The development of advanced materials for degrading organic dyes in wastewater has become a crucial focus in environmental remediation. This study synthesized quaternary FeBiZn selenide nanocomposites via a hydrothermal process to target the efficient degradation of dyes in aqueous media. The unique composition and structure of the nanocomposites resulted in enhanced photocatalytic performance under visible light. Detailed characterization using X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-Vis spectroscopy confirmed the successful formation and desirable properties of the material. The photocatalytic efficiency was tested on various dye pollutants, demonstrating significant degradation rates. The synergistic interaction of Fe, Bi, and Zn within the selenide matrix facilitated better charge separation, extended light absorption, and improved photocatalytic activity. This work highlights the potential of FeBiZn selenide nanocomposites as a sustainable solution for the removal of harmful dyes from wastewater, contributing to cleaner water systems

Keywords: FeBiZn selenide; nanocomposites; hydrothermal synthesis; photocatalysis; environmental remediation

Fabrication of CuO-NiO and PLN/CuO-NiO Bimetallic Composites for the removal of Imidacloprid Pesticide

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Imidacloprid (IMI) is one of the most commonly used insecticide specially used to control pests in agriculture. It is carcinogenic, mutagenic and have negative impact on endocrine system and disturb the life of aquatic organisms. The aim of the current research was to synthesize copper oxide nickel oxide (CuO-NiO) by coprecipitation method and polynidole copper oxide nickel oxide (PLN/CuO-NiO) bimetallic composites via in situ-polymerization process. The optical properties, percentage crystallinity, functional group, surface morphology and elemental composition were determined through UV-Visible spectroscopy, X-ray diffraction, Fourier transform infrared spectroscopy, Scanning electron microscopy and Energy dispersive x-ray spectroscopy, respectively. A photodegradation approach was adopted to eliminate IMI from wastewater by optimizing various process parameters including pesticide concentration, composite dose, effect of pH, exposer time and oxidant dose. The highest degradation efficiency of IMI obtained was 91 % using PLN/CuO-NiO. Rate and mechanism of degradation was studied by applying kinetic models and it was seen that Behnajady-Modirshala-Ghanbery model fitted the best on the experimental data. Stability and reusability of the prepared composites was checked in a five number of cycles and it was concluded that the degradation efficiency was decreased from 91 to 35 % by PLN/CuO-NiO. Therefore, these bimetallic composites have proven to be best for the degradation of IMI pesticide as well as for the remediation of wastewater on commercial scale.

Keywords: Imidacloprid, Bimetallic composite, Polyindole, Photocatalysis, Visible light

First principle study of PTO based porous extended conjugated polymer of high potential as a cathode material for Mg-ion batteries

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Magnesium-ion batteries (MIBs) can address the demand of large-scale energy owing to huge abundance of Mg in nature and higher superiority in energy density for next generation but its practical application halt due to complexity of its chemistry. Herein, we report first time pyrenetetraone and 1,3,5-tribromobenzene based extended conjugated porous polymer as cathode material for Mg-ion batteries applying density functional theory. Pyrenetetraone porous extended conjugated polymer (PTOPECP) highly stable dynamically and thermodynamically with strong affinity of Mg-ion with redox-active (C=O) due to narrow HOMO-LUMO energy gap which shows semiconductor nature. The binding energy (*BE*) for first and second Mg-ions found -3.62918 and -3.43171 eV, respectively. Single porous unit of **PTOPECP** loaded with twelve (12) Mg-ions between each redox-active (C=O) groups exhibiting low positive open circuit voltage 1.62 eV, high specific theoretical capacity of 320.0177 mAh/g, and with low energy barrier of 0.049 eV. No structure distortion in **PTOPECP** found prior and after fully loaded Mg-ions. Our results suggest that extended conjugated **PTOPECP** as promising cathode material for Mg-ion batteries in coming.

Study of Polystyrene and Cement Composites; Their Application as a New Construction Material

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Polystyrene and cement composites posses characteristics such as low density and high strength as compared to its weight. This study aims in assessing the utilization of polystyrene grains which are better known as Styrofoam, as an aggregate in cement blocks that have low density. Different experiments are conducted with the varying ratio of cement. The resulting composites exhibit good properties, but the durability and compressive strength is somewhat compromised due to the use of low weight polystyrene that has very less strength. The observation is made from studies with the increase in polystyrene content, the compressive strength seemed to be decreased while thermal resistance is also increased. The density of composites produced, varies from 810 kg/m^3 to 1140 kg/m^3. The thermal conduction of composites manufactured ranges from 0.14 to 0.31 W/mK while the maximum compressive strength came out is 3.12 N/mm^2. Key outcomes revealed that the concrete containing cement and polystyrene exhibit properties which make it a potential user as light weight filling applications for construction due to its mechanical, thermal and transport properties.

Keywords: Polystyrene Cement composites, Compressive strength, Thermal resistance, Low density.

Flexible ITO Coated PET/Glass Based Thin PDLC Films using Diethyl Toluene Diamine (DETDA) Hardener

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Diethyl Toluene Diamine (DETDA) has been used as a hardener in conjunction with, thermotropic Nematic liquid crystal phase, polymer dispersed liquid crystal (PDLC) compounds, and thin films are maintained by using the starting-to-turn emulsification (PIPS) approach and a low birefringent-longitudinal yield. The effect of varying functional epoxy monomers was investigated and compared with both the doped samples and the PDLC flexible thin films. In PDLC manufactured with a 22% weight-per-cent ratio of nematic liquid crystal (NLC), the overall reaction time improves by 82% and the input impedance increases by 72%. When DEDTA hardener was utilized as a tacky glue agent hardener and they needed five hours to cure at 70°C. To find the perfect hardener ratio, PDLC films will also made using various concentrations of DETDA (hardener). When Diethylene toluene-di-amine (DEDTA) hardener was utilized as a tacky glue agent hardener, it was observed that reacted with epoxide to form a 3D cross-linked thermoset structure with the optical transparency and clarity of the picture in the ON state were noticeably improved. Although V_{th} and V_{sat} improve as the plastic mesh gets smaller, they improve as the polymer mesh continues to shrink, and as t_{off} rises as the copolymer mesh continues to shrink, the off-state penetration increases. The results have been demonstrated the dispersed condition of LC is well proportioned and that the transmittance variation reached its maximum value when the weight ratio of LC is 30% in PDLC and mol 3% of DETDA hardener. The visible light angular transmission of the PDLC film had improved according to its optical characterizations. In the meantime, we have been investigated that creating PDLC smart glass display technology with a low energy-efficient approach and good E-O qualities may be achieved by varying the hardener and mol% and LC content. The use of other window treatments and applications for installations, such as blinds, shades, and shutters, that don't provide nearly as excellent a performance and/or convenience as these switchable films, like electronic intelligent sustainable technology of thin PDLC smart film, can be significantly reduced.

Keywords: Thermotropic Phase, Intelligent PDLC Films, Diethylene toluene-di-amine, hardener, and sustainable technology.

Biogenic Synthesis of Zinc Oxide Nanoparticles Using NARC G1 Garlic (*Allium sativum*) Extract, their Photocatalytic Activity for Dye Degradation and Antioxidant Activity of the Extract

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The nanoparticles of zinc oxide (ZnO-NPs) were synthesized by the green method utilizing NARC G1 garlic (*Allium sativum*) plant extract. They were characterized by UV-visible, Particle Size Analyzer, SEM, XRD and FTIR. The spectra demonstrated the absorption peak at 370 nm and it is the ZnO-NPs distinctive band. The particle size determined by the Particle Size Analyzer was about 18 nm. The SEM confirmed the irregular morphology and XRD analyzed the hexagonal crystalline structure of NPs. The FTIR analysis peak at 570 cm^{-1} showed ZnO functional group was present. The photocatalytic activity for dye degradation under the presence of sunlight was observed. The crude concentrated extract yield recovered from different solvents ranged between 4.52-6.74 g/100g. The amount of total phenolic and flavonoid contents was obtained from the NARC G1 garlic ranging from 266-379 mg GAE/100g and 152-242 mg CE/100g. Aqueous ethanol showed the maximum extracting efficacy for the inhibition of linolic acid among other solvents. The finding of this research strongly highlights the importance of NARC G1 garlic bioactive components which can used in the nutrapharmaceutical industry. This research advocated the efficacy of the NARC G1 garlic (*Allium sativum*) plant as a green reducing agent for ZnO-NPs synthesis and the promising photocatalytic activity of these nanoparticles offers valuable applications for environmental remediation technologies.

Keywords: Green Synthesis, Nanoparticles, Dye degradation, Antioxidant activity

An efficient Fe_2Se_3/Fe_2O_3 Heterostructure Electrocatalyst for Oxygen Evolution Reaction

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In this study, novel iron-based electrocatalysts, including Fe_2Se_3, Fe_2O_3, and Fe_2Se_3/Fe_2O_3 heterostructures, have been developed to bring down overpotential in the oxygen evolution reaction (OER). Among these, the $Fe_2Se_3/$ Fe_2O_3 heterostructure emerges as a highly promising electrocatalyst for OER, offering exceptional efficiency, cost-effectiveness, and minimal overpotential. The Fe_2Se_3/Fe_2O_3 electrocatalyst exhibits outstanding electro-chemical performance, with a remarkable onset potential of 1.31 V (vs. RHE) and a minimum 160 mV over-potential at 20 mA/cm^2 for OER. Notably, this prepared electrocatalyst demonstrates the lowest overpotential when compared to benchmark Fe-based OER electrocatalysts. Furthermore, during controlled potential electrolysis at 1.65 V (vs. RHE), the electrocatalyst maintains a stable current density of 65 mA/cm^2, highlighting its impressive electrochemical robustness. The hydrothermal synthesis method used for the synthesis of Fe_2Se_3, Fe_2O_3, and their heterostructure is particularly very simple and straightforward. Which making them excellent candidates for water splitting applications, particularly in OER. These significant achievements accomplished through the utilization of non-precious metal electrocatalysts, open up new possibilities for practical OER implementations. Undoubtedly, these findings will greatly benefit the scientific community in the development of efficient electrocatalysts using non-noble metals for the electrochemical water splitting process.

Keywords: Oxygen Evolution Reaction (OER); Electrocatalysts; Fe_2Se_3/Fe_2O_3 heterostructure

Electrochemical sensing of dopamine on metal oxides modified glassy carbon electrode

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We report here the use of WO3, CuO, and WO3/CuO composite modified GC electrode for electrochemical sensing of DA in 0.1M PB solution having pH 7. The DA sensing materials (i.e.WO3, CuO and WO3/CuO composite) were synthesized via Hydrothermal method. The as synthesized materials were characterized by scanning electron microscopy (SEM) to examine the surface morphology, the crystallinity of the materials was checked using X-rays diffraction (XRD), and the functional groups and bonding were investigated using Fourier transform infrared spectroscopy (FTIR). These materials were fabricated on glassy carbon electrode (GCE) using drop cast method. The effects of DA concentration within the range of DA in the real blood were studied on WO3/GCE, CuO/GCE, and WO3/CuO/GCE using electrochemical technique cyclic voltammetry (CV). The effect of scan rate and point potential were also studied on all these electrode. The WO3/CuO composite modified GCE shows a high sensitivity having oxidation current (Ipa $\approx 2.07 \times 10^{-6}$ A) than WO3 having (Ipa $\approx 1.48 \times 10^{-6}$A) and CuO (Ipa $\approx 1.99 \times 10^{-6}$A) and also at lower potential. Differential pulse voltammetry (DPV) experiments were performed for determination of DA concentration in 0.1M PBS (pH 7), These experiments shows a broad linear concentration range from 10 μM up to 200 μM and the lower limit of detection were found to be 0.24 μM, the observed lowest detection limit over a wide concentration range of DA is due to the WO3/CuO/GCE possess better electrocatalytic activity and high electroactive surface area Effect of interfering species which co-exist with dopamine in the blood such as Asorbic Acid (AA), Glucose, NaCl, KCl etc were also studied via amperometry. It shows that each DA injection causes a significant increase in current, whereas the interfering species had no effect on current after their addition.

Keywords: Dopamine, Cyclic Voltammetry, DPV, Hydrothermal method

Optimization and validation of an analytical method for the analysis of seventy-seven pesticides in tomatoes using modified QuEChERS and LC-ESI-MS/MS

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The application of multiple pesticides of varying physiochemical properties on tomatoes its during short growing period raises significant concerns about potential consumers health. This necessitates the optimization and validation of a reliable analytical method for maximum residues limit compliance testing of pesticides. In this study, an analytical method for the analysis of seventy-seven pesticide used in tomato production was optimized and validated. The targeted pesticides were extracted using the citrate-buffered QuEChERS method, followed by cleanup with primary secondary amine (PSA) and graphitized carbon black (GCB). The extracted pesticides in trace amount were analyzed on LC-ESI-MS/MS in both positive and negative polarity modes. The method's accuracy for targeted pesticides ranged from 70.0 % to 119.7 %, with associated precision ranging from 0.85 % to 19.9 %. The method limits of detection and quantification were from 0.005 to 1.39 mg/kg and 0.01 to 4.17 mg/kg, respectively. The optimized method was applied to analyze 164 tomato samples collected from various agro-ecological regions, spanning from the mountains of Gilgit-Baltistan to the arid, dusty plains of Balochistan and Sindh. The validated method can be confidently used for pesticide residue compliance testing by pesticide residue testing laboratories, researchers, regulatory agencies, and food safety authorities.

Keywords: Pesticide residues, Tomatoes, modified QuEChERs, LC-ESI-MS/MS, Compliance testing.

A DFT Study of Synthetic Drug Aprocitentan: MEP, HOMO, LUMO, NBO and FUKUI FUCTION Analysis

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This study shows a detailed computational analysis of a synthetic drug Aprocitentan, with the IUPAC name N-[5-(4-bromophenyl)-6-{2-[(5-bromopyrimidin-2-yl)oxy]ethoxy}pyrimidin-4-yl] sulfuric diamide. The molecular structure of Aprocitentan was optimized using Density Functional Theory (DFT) at the B3LYP/6-31G(d) level of theory. Some key structural parameter like bond angles, bond lengths and dipole moment (4.293574) are revealed by optimized geometry. The electronic properties, such as the HOMO-LUMO gap (4.927 eV), electron affinity (1.392 eV) and ionization potential (6.319 eV) indicate the molecule stability and low reactivity. The Natural Bond Orbital (NBO) analysis show significant electron delocalization contributing to the Aprocitentan molecule stability. Furthermore, the Fukui Function study across anionic, neutral and cationic states highlighted varying reactivity sites, with bromine atoms showing high nucleophilicity in the anionic state and specific carbon atoms being more reactive under electrophilic conditions. These findings provide a comprehensive understanding of Aprocitentan's chemical stability, reactivity and potential behavior in different chemical environments.

Keywords: DFT study; Aprocitentan molecular study; DFT study of aprocitentan; Molecular simulation

Synthesis of poly GG-co-AAm-co-MAA; A terpolymer hydrogel for the removal of methyl violet and fuchsin basic dyes from aqueous solution

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A novel adsorbent designated as ter-polymer hydrogel (gellan gum-co-acrylamide-co-methacrylic acid) was prepared by free radical polymerization of gellan gum (GG), methacrylic acid (MAA) and acrylamide (AAm) using MBA (N, N-methylene bis-acrylamide) as crosslinker and ammonium per sulfate (APS) as initiator of reaction. The synthesized gel was characterized by SEM, FTIR, XRD, BET and TGA, and was used for the adsorptive removal of Methyl violet (MV) and Fuchsin Basic (FB) dyes from aqueous solution. The effect of temperature, contact time, pH, and concentration on them under study adsorption process was evaluated. Freundlich isotherm and pseudo-second-order kinetic models were found best in fitting the isothermal and kinetics data. The water diffusion and % swelling of hydrogel was studied at various pH in distilled water and at neutral pH in tap water. The diffusion was found to be of Fickian type with maximum swelling of 5132%. The maximum adsorption capacity was 233 mg/g against MV and 200 mg/g against FB dyes. The swelling, and adsorption were pH dependent and increased with increase in pH. The enthalpy, Gibbs free energy and entropy changes of adsorption for both the dyes indicated the adsorption process to be exothermic, feasible, and spontaneous. The hydrogel was successfully regenerated using acetone and distilled water for five cycle and still its dyes removal efficiency was 80% of its original value. The poly(GG-co-AAm-co-MAA) hydrogel successfully removed the selected dyes from water and could thus be used as an efficient alternative sorbent for cationic dyes removal from aqueous solutions.

Keywords: Hydrogels; Swelling; adsorption; thermodynamics

Spectroscopic Studies of the Interactions of Bisphenol A with Cetyltrimethyl Ammonium Bromide

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BPA is an endocrine-disrupting chemical used in different industries. BPA is released into the environment from different sectors and thus pollutes the environment. Surfactants can improve the solubility of the nonpolar compounds in water. BPA is less soluble in water, therefore CTAB can improve the solubility of BPA in water. Studying the interactions is an important parameter to know about the best possible materials for removal. In the current literature, no study is available about the effect of pH on the interactions of BPA with CTAB. Above pK_a BPA ionizes which affects the interaction behavior of BPA with CTAB. Here in this work, the interactions of BPA with CTAB are studied at different pH using UV-Vis spectroscopy. The binding constant (K_b), partitioning constant (K_c), and Gibbs free energies (ΔG_b and ΔG_p) are determined using UV-Vis spectroscopy. The K_b and K_c values increase with an increase in pH showing that the interactions become stronger with the increase in pH of the solution. At higher pH, BPA can interact with the head group as well as with the hydrophobic part of surfactants. Gibb's free energy shows that the process is spontaneous. This study can play an important role in the removal of BPA through surfactants.

Keywords: Surfactants; interaction; Bisphenol A; spectroscopy

Synthesis and Bioactivity Evaluation of 3-Ethoxy-4-Hydroxybenzaldehyde Based-Benzimidazole Derivatives

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This study outlines are multistep synthetic route for the synthesis of benzimidazole derivatives, a class of compounds renowned for their diverse applications in medicinal chemistry. The synthesis commences with the esterification of 3-Ethoxy-4-hydroxybenzaldehyde employing methyl bromoacetate. It is an essential initial step for introducing the necessary functional groups for subsequent reactions. Following esterification the resultant compound undergoes condensation with *o*-phenylenediamine facilitating the formation of the benzimidazole nucleus which is a fundamental structural moiety in many bioactive molecules. Continuing the synthetic pathway, hydrazine is employed to effectuate the conversion of the ester group within the benzimidazole structure into a hydrazide moiety. This strategic modification not only enhances the chemical diversity of the synthesized compounds but also presents opportunities for further functionalization and diversification of the molecular structure. In the final step of the synthetic sequence the synthesized hydrazide is subjected to reaction with an array of aromatic and aliphatic aldehydes providing a diverse class of imine derivatives. The elucidation of the molecular structures of the synthesized compounds is achieved through modern spectroscopic techniques including 1H and 13C NMR Spectroscopy to ensure the accuracy and reliability of the synthetic route. This comprehensive synthetic approach offers a versatile platform for the systematic exploration and development of novel benzimidazole derivatives with specific properties suitable for many applications.

Green Synthesis, Characterization of ZnO Nanoparticles and its Conjugates Prepared with Thalidomide and Biological Activities

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Thalidomide drug having anti-angiogenic, anti-inflammatory, immunomodulatory, anticancer, hypnosedative and antiemetic actions but has some teratogenic effects. In this research zinc oxide nanoparticles (ZnO-NPs) were prepared by green method from the *Rhazya stricta* plant, and then conjugated with thalidomide drug. The preparation of ZnO-NPs and its conjugates were confirmed by using different characterization technique i.e UV-Vis spectroscopy (UV-Vis), Fourier transform infrared spectroscopy (FTIR) and X-Ray diffraction (XRD) analysis. The anticancer activity was carried out of various doses of Thalidomide and its conjugates by evaluating their influence on cell viability. The highest potency was shown by the 2ZT (2:1) which revealed an average survival of UG-87 cells was 24.02% in the lowest concentration being 100 µL, whereas it further decreased to 20.04% at 200 µL. This study suggests that these conjugates can be useful in increasing the efficacy of drugs at relatively low concentrations. So, it is recommended to work on the mechanism and toxicity of these conjugates.

Keywords: Thalidomide; *Rhazya stricta*; anticancer; UG-87 cells

Chemical fingerprinting, *in-vitro* and *in-silico* antioxidant and anti-aging potential of *Crocus sativus* (Saffron)

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Skin aging is a complex, inevitable biological phenomenon. Overproduction of reactive oxygen species (ROS) and extracellular matrix-degrading enzymes contribute to aging. This study aimed to explore Crocus sativus L. saffron antioxidant-mediated antiaging potential in order to determine its efficacy in protecting skin against ROS-induced damage through in vitro and in silico analysis. Saffron was evaluated for its antioxidant potential through in vitro DPPH and ABTS assays. While inhibition of tyrosinase, elastase, and hyaluronidase enzymes assessed its anti-aging potential. LCMS analyses explore its active phytoconstituents, and Swiss ADME analyses predict its skin permeability potential. Molecular docking and MDS analysis against target proteins assess binding potential and stability in the enzyme molecular pocket. Saffron showed significant antioxidant and anti-aging potential with 74.24±1.84 µg/mL flavonoids content and 27.03±1.6% elastase inhibition. LCMS analysis revealed the presence of several pharmacologically beneficial phytochemicals, including crocetin, zeaxanthin, fucosterol, b-sitosterol, stigmasterol, safranal, methylparaben, and benzoic acid, identified as skin permeable and effective anti-aging constituents. Stigmasterol, with a binding energy of -16.5871 kcal/mol against elastase, emerges as the most promising candidate for antiaging potential. Molecular dynamic simulation at 100 ns further confirms the stability and effectiveness of saffron in dermatocosmetics applications. Saffron demonstrated strong antioxidant and antiaging potential. In vitro and in silico analyses indicate their promising role in skin care and cosmetics, with further clinical trials required to validate their anti-aging potential through in vivo analysis.

Keywords: Anti-oxidant, anti-aging, dermatocosmetics, in-vitro, in-silico

Synthesis, Bioactivity and Photophysical Property of Benzophenone *Bis* Schiff Bases

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Among the valuable structures in chemistry, Schiff bases have essential importance as multi-oriented scaffolds. Such compounds are widely used as starting substances for chemical transformation and synthesizing biological active compounds. Schiff bases are good ligands for transition metal complexes which possess many biological activities including antimalarial, antibacterial, antifungal, antiviral, anti-proliferative, antipyretic, and antiprotozoal properties. Synthesis, bioactivity and photo-physical properties of benzophenone based bis Schiff base derivatives have opened a window in synthesis and drug design field. In view of the massive importance and extensive applications of *bis*-Schiff bases, the recent study has been planned to synthesize and assess the medicinal and photo-physical aspects of *bis*-Schiff base derivatives based on benzophenone. In present research work, we have synthesized different bis Schiff base derivatives of benzophenone. First, benzophenone was reacted to hydrazine hydrate to give imine. It will be further treated with a series of carbonyl compounds to furnish the titled bis-Schiff base derivatives. The target compounds were characterized through UV, FT-IR and 1 HNMR. After structure conformation, they will be evaluated for their biological activities such as anti-microbial and antioxidant through established protocol. In-silico studies were conducted to investigate the potential binding interactions between the newly synthesized compounds and cyclooxygenase (COX-II). Out of the eighteen synthesized compounds, four exhibited higher binding scores than the standard reference used. These four compounds were subsequently evaluated for their In vivo anti-inflammatory activity and were found to be active.

Synthesis and Characterization of Nitro-Substituted Polyhydroquinoline Derivatives

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This research study presents the synthesis and characterization of Polyhydroquinoline derivatives based on 4-Nitrobenzaldehyde. Various imine derivatives of 4-nitrobenzaldehyde-based Polyhydroquinoline (PHQ) were synthesized through a three-step process. In the first step, PHQ was synthesized via the Hantzsch reaction. The second step involved the reduction of the nitro group in 4-nitrobenzaldehyde-based PHQ to produce 4-aminobenzaldehyde-based PHQ. In the final step, 4-aminobenzaldehyde-based PHQ was reacted with different substituted benzaldehydes to yield the desired acyl imine derivatives. The structures of the synthesized compounds were confirmed using a range of experimental techniques and modern spectroscopic methods. Additionally, the synthesized compounds were evaluated for their antimicrobial, antifungal, antidiabetic, and antioxidant activities.

Synthesis, Evaluation of Biological Activities, and Molecular Modeling of Ketoprofen Derivatives

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This research presents a comprehensive investigation into the synthesis, characterization, and anti-inflammatory activities of imine derivatives of ketoprofen acid, both *In-silico* and *In-vivo*. The imine derivatives were synthesized through a two-step process. In the first step, ketoprofen acid was chemically modified to form ketoprofen acid hydrazide using carbonyl diimidazole (CDI) and hydrazine hydrate. In the second step, the ketoprofen hydrazide was reacted with various substituted benzaldehydes to obtain the desired imine derivatives. The structures of the synthesized compounds were confirmed using 1H-NMR spectroscopy. *In-silico* studies were conducted to investigate the potential binding interactions between the newly synthesized compounds and cyclooxygenase (COX-II). Out of the eighteen synthesized compounds, four exhibited higher binding scores than the standard reference used. These four compounds were subsequently evaluated for their *In vivo* anti-inflammatory activity and were found to be active.

Structural features, dielectric and magnetic properties Yb-ion substituted Co-Zn spinel ferrites

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Yb^{+3} doped Co-Zn based spinel ferrites composition Co0.5Zn0.5YbxFe2-xO4 are synthesized via sol-gel method and characterized by XRD, FTIR, SEM, Impedance Analyzer and VSM. The phase analysis revealed a cubic spinel structure having a single phase. Similarly, XRD peaks became less intense and their width became larger with Yb+3 substitution due to the larger ionic radius of Yb3+ (0.99 Å), comparative with the ionic radius of Fe+2 (0.645 Å). The M-O vibrations at octahedral and tetrahedral sites are confirmed by FTIR spectra. Dielectric parameters are carried out using impedance analyzer within frequency range 60 Hz - 110 MHz at room temperature. Dielectric constant is significantly affected with Yb3+ and attained 2903 value at 36 MHz for Co0.5Zn0.5Fe1.948Yb0.052O4. Furthermore, Co0.5Zn0.5Fe1.948Yb0.052O4 showed dielectric loss of -1802 at 36.1 MHz. The saturation magnetization, remanence, and coercivity confirmed the soft magnetic nature of the material. Excellent dielectric and magnetic properties of material suggested that they are best for high-frequency devices, super-capacitors, sensing, isolators, data storage and energy storage devices.

Keywords: Spinel ferrites; Sol-gel; XRD; FTIR; Dielectric Constant; Electric Modulus; Cole-Cole plots; Grain boundary contribution

Alkaline Fusion Assisted Synthesis of K-Zeolite from Rice Husk for Wastewater Treatment

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In recent years, water sustainability has become one of the foremost research areas in the field of environmental protection. The treatment of recalcitrant organic pollutants in water is challenging by conventional techniques. According to recent studies, cleaning up organic pollutants via a photocatalytic technique is highly recommended. Massive generation of carcinogenic fly ash waste poses major hazards to environment due to its discharge into drains and landfills. In this research work to address rice husk fly ash related problems the waste was being modified and reused using an incredibly quick non-conventional waste management protocol to produce value-added products. The modification of rice husk fly ash into zeolite was accomplished by alkaline activation, via an advanced hydrothermal strategy. The evaluation of modified material regarding their morphology, surface porosity, chemical composition, functionality, mineral phases, and crystallinity was done by Scanning electron microscope (SEM), Fourier transform infrared spectroscopy (FTIR) X-ray diffraction spectroscopy (XRD) and inductively coupled plasma atomic emission spectroscopic (ICP-AES) techniques. synthetic materials showed excellent zeolitetaion characteristics and ion exchange capacity which is responsible for their applications related to wastewater treatment. In order to access the applicational capability of synthetic zeolites, their metal purging activity was performed at laboratory level to remove Zn (II) from synthetic wastewater. The reaction parameters, such as the starting metal ion concentration, mass of the adsorbent, sorption time, and pH of the reaction medium, were varied throughout the activity. This research leads to the conclusion that the transformation of coal fly ash waste into value-added zeolites for wastewater treatment may represent an emerging step toward attaining sustainable and environment friendly remediation.

Investigation of Optical Properties and Wettability of Chitosan/Silica Composite Films

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This work presents an investigation of optical and wettability properties of chitosan/silica composite films. Silica nanoparticles were dispersed into chitosan matrix and the composite films were obtained via solution casting method. The synthesized films were physiochemically characterized through Fourier Transform Infrared (FTIR) spectroscopy and X-Ray Diffraction (XRD). UV-Visible spectroscopy was employed for the measurement of UV-visible absorption, transmittance, refractive index and band gap energy to understand optical behavior of composite films. Optical dielectric properties including optical conductivity, dielectric constant and dielectric loss were also calculated. Contact angle and surface energy of films were measured to find the wettability of films. All composite films had higher UV screening ability and wettability than pure CS film. The refractive index and optical dielectric properties were found to vary with the composition of the films. The calculated band gap energy provided insights into the electronic structure of the composites. The results show that CS/SiO_2 composite films possess tunable optical properties and have potential applications in biodegradable optoelectronic devices.

Keywords: Chitosan; Silica; Bionanocomposite; Optical Properties.

Reverse Osmosis Technology: A Possible Solution to Global Water Scarcity

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The availability of good quality drinking water is one of the burning issues of the modern industrialized world. The available freshwater reservoirs are no longer sufficient to fulfill the drinking water requirements of the day-by-day increasing population of the world. Therefore, the emphasis is shifting to the utilization of brackish and marine water reservoirs for the production of quality drinking water through the desalination process. The reverse osmosis technology has emerged over the last few decades as the leading method for the production of potable water via desalination of brackish and seawater. This paper covers the technical, financial, and environmental aspects of reverse osmosis desalination. Furthermore, the industrial applications of reverse osmosis technology in Pakistan and future research needs for improving its efficiency and cost-effectiveness are also elaborated.

Single-Step Synthesis of Co/Ni/Cu Trimetallic Nanoparticles and Photocatalytic Purification of Water

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Water pollution is a severe threat and causes harmful effects on the ecosystem, human health and the environment. Water pollutants are causing serious illnesses like cancer and severely affecting aquatic plants and animals. Overcoming issues caused by water pollution is essential to ensuring our ecosystems' sustainability, improving human health, and preserving water quality for the future. This research work focuses on designing and synthesizing ternary metallic composites and their use for the degradation of organic water pollutants. Here, through the chemical reduction method, Co/Ni/Cu ternary nanoparticles have been prepared. UV-visible and FTIR Spectroscopy have been used to monitor the synthesis process of nanoparticles. These synthesized nanoparticles have been further employed for the catalytic degradation of organic dye, methylene blue. UV-visible spectroscopy has been used for the degradation study of methylene blue. Reduction in intensity of the peak of the VU-Visible spectrum of methylene blue corresponds to degradation of dyes. The results of the catalytic degradation of methylene blue are quite impressive and encourage the use of such metallic nanoparticles for the removal of organic pollutants from water.

Keywords: Water Treatment; Trimetallic; Catalysis

Fabrication of Co_3O_4 and Co_3O_4-Cu-BTC based Electrochemical Sensor for Voltammetric Determination of Toxic Cadmium ions

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The performance of the Co_3O_4 (CoCPE) and Co_3O_4-Cu-BTC (CoBCPE) modified carbon paste electrodes was evaluated for the differential pulse voltammetric detection of toxic cadmium ions in aqueous solutions. The cobalt oxide nanoparticles were prepared through solvent deficient method and modified with copper-benzene tricarboxylic acid (MOF) via layer-by-layer assembly. Both simple and modified cobalt oxide nanoparticles were structurally characterized by FTIR, pXRD, SEM, EDX, BET, TGA and 4-point probe method. The modified carbon paste electrodes were then fabricated as electrochemical sensors with the synthesized materials via a slurry paste method. Electrochemical characterization of the electrodes was conducted using EIS and CV in a K3[Fe(CN)6] solution, revealing charge transfer resistances of 20.06 Ω for CoCPE and 7.69 Ω for CoBCPE. The electrochemical surface areas were determined to be 3.51 cm^2 and 4.61 cm^2 for CoCPE and CoBCPE, respectively. Various experimental parameters, including the amount of modifier, accumulation medium, concentration and pH of the accumulation medium, deposition time, deposition potential, and cadmium ion concentration, were optimized to enhance sensitivity. Detection limits were found to be 0.095 mg/L for CoCPE (5 %) and 0.069 mg/L for CoBCPE (1 %), demonstrating that the Co_3O_4-Cu-BTC-modified material provided superior performance. These findings suggest that the modified material achieves a lower detection limit even with a 5 % smaller amount. The excellent reproducibility of the results suggests the potential for developing electrochemical sensors based on Co_3O_4 and Co3O4-Cu-BTC for routine cadmium ion analysis in aqueous solutions.

Keywords: Cobalt Oxide; Electrochemical Sensor; Cadmium ions; Differential Pulse voltammetry

Chemo-selective Hydrogenation of Carbonyl Compounds over Bimetallic Catalysts

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Selective hydrogenation of carbonyl moiety in the presence of olefinic group and other reducible functionality is an industrially important transformation. However, the protocol of green chemistry cannot be sacrificed for this formidable challenging transformation. Therefore, iron nickel bimetallic recyclable catalyst (Fe/Ni) was used for base free hydrogenation of carbonyl compound with high activity and chemoselectivity in microwave environment. The microwave irradiation and pre-treatment of bimetallic catalyst (Fe/Ni) divert conversion/selectivity toward C=O group as compared to C=C or another reducible moiety. This is further confirmed by DFT calculations which shows that the C=O site is strongly interacted with the surface compared to the C=C site. The pyridine adsorption studies revealed that pre-treated (Fe/Ni) possess more acidic sites as compared to untreated catalyst. Furthermore, the selectivity of bimetallic catalysts towards hydrogenation of carbonyl function group was correlated with Fe content present in the matrix of catalyst.

Keywords: Bimetallic catalysts, microwave, hydrogenation, Carbonyl compound

Innovative Ni-Based Metallic Foams: A Pathway to Sustainable Hydrogen Production through Water Splitting

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The depletion of fossil fuels has positioned hydrogen production as a compelling alternative for sustainable and eco-friendly energy. Electrochemical water splitting is widely regarded as the most effective method for hydrogen production. However, electrochemical water splitting presents significant energy challenges. Therefore, designing a cost-effective, abundant, and eco-friendly electrocatalyst is a key focus. In this study, we report the development of self-grown NiCo, NiCu binary oxides and NiO/MnS composites on nickel foam for the oxygen evolution reaction (OER) in electrochemical water splitting under alkaline conditions. The catalysts were synthesized using a simple one-step hydrothermal method followed by calcination. Morphological analysis revealed finely shaped nanoparticles, while X-ray diffraction (XRD) confirmed the presence of crystalline phases. Fourier transform infrared spectroscopy (FTIR) verified the formation of metal-oxygen bonds. The synthesized NiCo binary oxides and NiO/MnS composites exhibited low overpotentials of 320 and 260 mV at 50 mA/cm^2 for OER. The NiCu prepared at 24 hours displayed overpotential of 390 mV to achieve a current density of 10 mA/cm^2. Durability tests conducted over 1000 CV cycles demonstrated their stability and effectiveness. These catalysts show great promise for OER in electrochemical water electrolysis, making them crucial for hydrogen fuel generation.

Key words: Hydrothermal, water splitting, electrochemical water splitting, hydrogen production, binder free growth

Synthesis, Characterization of Biocompatible Iron Oxide Nanoparticles Drug Conjugates with Thalidomide: An Alternate to Boost the Anti-inflammatory and Alkaline Phosphatase Assays

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Thalidomide was initially used as sedative, later its Anti-inflammatory aspects was also explored and within no time becomes the medicine of choice in morning sickness condition. Later it faced a serious controversy with respect to its use as was declared banned from the market because of associated birth defects in new born babies. In COVID-19 it was picked once more for its potential use as anti-inflammatory drug except for pregnant women. The chiral centers and other active sites extend its use as anti-cancerous agent on other side consequently, make it a better choice as anti-inflammatory cum anticancer drug. Just like other recommended medicines as anticancer it suffers with an issue of side effects. To minimize these side effects and have promising results the thalidomide was used in conjugation with a nano-carriers, iron oxide. The iron was used as nano-carrier because it plays pivotal role in cancer cell abnormal growth and very important for the development of potential strategies for tumor treatment. Therefore, to exploit the pharmacological benefits of thalidomide and the role of iron in cellular function, this effort focuses on iron oxide nanoparticles (FeO-NPs) and iron oxide thalidomide conjugates (FeO-Th) conjugates synthesis in different ratios. The synthesized formulations were characterized by SEM, XRD, FTIR and UV-Visible spectroscopy. The efficacy of these characterized conjugates was evaluated through *in vitro* and *in vivo* procedures using anti-inflammatory and alkaline phosphates enzyme assay. In, *In vitro and in vivo* anti-inflammatory of our tested formulation has almost equal inhibition of BSA denaturation compared to the standard used. Using the alkaline phosphatase test, the same conjugates exhibited the strongest suppression. Therefore, FeO-Th conjugates appears to possess stronger anti-inflammatory effects and higher inhibition towards alkaline phosphatase, can be potential candidates for treating as has the ability to reverse the tumor microenvironment and can stop cancer cells growth.

Keywords: Thalidomide, Iron Oxide, Drug Conjugates, Anti-inflammatory, Anticancer.

Dicarboxamide Derivatives of Salicylic Acid: Synthesis, Characterization and Biological Activities

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In this study, dicarboxamide derivatives of salicylic acid were synthesized using a three-step process. In the first step, salicylic acid was converted to methyl salicylate, which was then transformed into salicylic acid hydrazide in the second step. In the final step, salicylic acid hydrazide was reacted with various acyl halides to obtain the targeted dicarboxamide derivatives. The structures of the synthesized compounds were confirmed using 1H-NMR spectroscopy, and for additional confirmation they are submitted for 13C-NMR and mass spectrometry. These compounds have been successfully submitted for evaluation of their anti-inflammatory, analgesic, and antipyretic activities.

Characterization of humic acid from Thar coal mines Sindh, Pakistan

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This study explores the potential of humic acid (HA) extracted from lignite coal in Pakistan to enhance agricultural productivity and soil health. Despite Pakistan's rich coal reserves, the low quality of its coal, characterized by high ash and moisture content, limits its use as fuel. However, research indicates that the crumbled lignite coal contains significant amounts of humic acid, which is essential for improving soil structure and promoting plant growth. Humic acid is known for its ability to chelate nutrients, enhance mineral uptake by plant roots, and improve soil fertility. By utilizing HA as a natural fertilizer, this research aims to reduce reliance on chemical fertilizers, boost crop yields, and mitigate soil degradation. The findings suggest that integrating humic acid into agricultural practices can lead to sustainable farming solutions in humus-deficient soils, particularly in the Thar region of Pakistan. The extraction process involved using four different concentrations of Na4P2O7.H2O, KOH, and NaOH (1%, 2.5%, 3%, and 3.5%). Among all concentrations, the 3.5% samples proved optimal for humic acid extraction, yielding 32.25% from NaOH, 19.99% from KOH, and 15.54% from Na4P2O7.H2O. By utilizing HA as a natural fertilizer, this research aims to reduce reliance on chemical fertilizers, boost crop yields, and mitigate soil.

Microbial Models for *in vivo* Drug Metabolism

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Drugs, taken through various means, undergo extensive metabolism upon interaction with the body enzyme system, leading to the formation of variety of metabolites. Identification and characterization of these metabolites is of utmost importance to know about the possible effects they might have on the body. Over the past few decades, microbial biotransformation has developed as a technique for structural modification of organic compounds, employing the microbial enzyme systems. Biotransformation of marketed drugs, in most cases, has led to the synthesis of products, already identified as *in vivo* metabolites of the same drug. Thus, the technique can be used effectively for the biotransformation of bioactive compounds or possible lead molecules. This would provide an overview of the probable metabolic pathway and metabolites, possibly produced inside the body, upon ingestion. In this context, microbial transformation of several steroidal drugs was carried out, leading to the formation of products, some of which have already been identified as *in vivo* metabolites, making these microbial strains potential models for *in vivo* metabolism of drugs.

Keywords: Microbial biotransformation, Metabolism, Drugs, Biocatalysis

Characterization and biofabrication of isolated silver nano particles with humic acid and their role against test pathogens causing skin infections

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In modern research, nanotechnology is the current area ofmaterials science. In medical technology, the application ofsilver nanoparticles (AgNPs)has a wide range, which gives scopefor further research in the field of fabrication of silvernanoparticles Biosynthesis of silver nanoparticles is gaining significant importance due to environmentally safe and it is an efficientalternative method. It isalready known that silver has been used as an antimicrobialagent for centuries, in the present days the repetition ofantibiotics increasing threat of antibiotic resistance, causedby the exploitation of antibiotics. So, Scientists once againfocus on the application of AgNPs. In the present study, silver nanoparticles were synthesized by using silver nitrate salt and humic acid (HA) was isolated from cow dung by IHSS method, the synthesized NPs were then coated with HA. The AgNPs, HA and fabricated AgNPs-HA were characterized by spectral analysis; the UV-Vis spectral peak of AgNPs showed maximum absorption at 445 nm. Fourier-transform infrared spectroscopy (FT-IR) data show that the O–H hydroxyl groups, carboxylic acids, ester and ether groups and C–O stretching of alcohols have been utilized in the formation and fabrication of AgNPs. The X-ray powder diffraction (XRD) data reveal that the AgNPs are face-centered cubic (fcc) in structure. The size was determined by particle size analyzer and atomic force microscope (AFM); the results reveal that AgNPs were spherical in shape and the average grain size is determined as 41.5–46.5 nm. The biofabricated AgNPs are extremely stable due to its high negative zeta potential indicates that the nanoparticles are polydispered in nature.

Keywords: Biofabrication, Silver nanoparticles, Humic acid, Pathogens.

Synthesis of zinc oxide based etoricoxib and montelukast nanoformulations and their biomedical applications

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The current study described the synthesis of novel low dose PVA capped Etoricoxib (ET) and montelukast (MT) conjugated Zinc Oxide (ZnO) nanomaterials (NMs) as potential anti-inflammatory, analgesic and antipyretic agents. A facile coprecipitation protocol was used for synthesis of NMs by combination of ET, MT and ZnO NP. The efficient synthesis of ET and MT conjugated ZnO NMs were confirmed through UV–visible, XRD, FTIR and DLS analysis. Data of in vivo anti-inflammatory activity indicated that potency of ZnO NMs was found to be greater than drugs (ET and MT). Analgesic potency of NMs was much higher than that of drugs (ET and MT). The in vivo antipyretic activity indicates that the results of NMs and drugs (ET and MT) are of similar effect but that of NMs are more potent based on per weight basis. A wide therapeutic window was shown by the acute toxicity study carried out via LD50 method. It is concluded that the novel low dose PVA capped ET and MT conjugated ZnO NMs were potential analgesic, antipyretic and anti-inflammatory agents.

Keywords: Zinc oxide nanoparticles, Etoricoxib, Montelukast

Novel pH-Responsive Peptide-Paclitaxel Conjugate with Improved Therapeutic Potentials against Glioblastoma

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The development of peptide drugs has made tremendous progress in the past few decades because of the advancements in modification chemistry and analytical technologies. The novel-designed peptide drugs have been modified through various biochemical methods with improved diagnostic, therapeutic, and drug-delivery strategies. Furthermore, the emergence of peptide-drug conjugates (PDCs)—utilizes target-oriented peptide moieties as a vehicle for cytotoxic payloads via conjugation with cleavable chemical agents, resulting in the key foundation of the new era of targeted peptide drugs. The cell-penetrating peptide (CPP = c[RGDKLAK]) is an effective, short-chain dual-targeting cyclic heptapeptide probe that consists of both tumor-homing motifs (RGD) coupled with a proapoptotic motif (KLA). This peptide probe can specifically interact with $\alpha_v\beta_3$-integrin receptors highly expressed on endothelial cells as well as many types of tumor cells, most specifically brain tumor glioblastoma cells. To improve the specificity, hydrophobic nature, selectivity, and therapeutic efficacy of paclitaxel, it was conjugated with CPP through succinic acids linker moiety via covalent/ ester bond. It was also observed that PTX is released from PDC in its active form until internalized into cancer cells because of the chemical nature of the ester bond (covalent linkage). The resultant PDC showed promising tumor-growth inhibitory effects (> 3-folds) of PDC in brain tumor-bearing mice models. Subsequently, our findings confirmed that the novel-designed PDC (CPP−SA−PTX) adduct may serve as a promising therapeutic agent to treat glioblastoma.

Keywords: Peptide-Drug Conjugates; Chemical Biology; Cell-penetrating Peptide; Cytotoxic Payloads.

HIV-1 replication: fidelity, drug resistance and unexploited antiviral targets

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Reverse transcriptases (RTs) are nucleic acid polymerases that synthesize DNA using RNA or DNA as templates, while degrading RNA when forming RNA/DNA hybrids (RNase H activity). RTs play a pivotal role in the replication of several virus families, most notably *Retroviridae* and *Hepadnaviridae*. These enzymes are devoid of proof-reading activity and contribute to the large variability observed in human immunodeficiency viruses (HIV), with intrinsic error rates of 10-4 to 10-5, a fact that explains in part the enormous genetic variability observed in HIV-1. In addition, RTs are widely used for research and biotechnological applications that require cDNA synthesis, including RT-qPCR and high-throughput RNA sequencing (RNA-seq). A main goal in generating RT mutants suitable for transcriptomics and gene expression analysis is to achieve higher optimal temperature and thermal stability, higher processivity and increased catalytic efficiency. Recent work carried out in our lab reveals that the RT's RNase H activity has a major impact on DNA polymerization during the reverse transcription process (Luczkowiak *et al.*, 2018, *J. Biol. Chem.* 293, 13351; Martín-Alonso *et al.*, 2022, *J. Mol. Biol.* 434, 1677507; Martínez del Río *et al.*, 2023, *J. Mol. Biol.*, 435, 168219). On the other hand, HIV-1 RT inhibitors acting on its DNA polymerase activity constitute the backbone of currently prescribed antiretroviral therapies. Despite the efficacy of these therapies in controlling HIV replication, the increased prevalence of drug resistance in some regions of the world anticipates the need of novel antiretroviral drugs targeting resistant HIV strains. I will review our recent efforts to understand RNase H function in reverse transcription and how RNase H mutational inactivation affects DNA-dependent DNA synthesis fidelity, template switching and strand displacement. In addition, I will discuss our recent work on the characterization of novel active site RNase H inhibitors, including coumarin derivatives with dual inhibitory activity against RT DNA polymerase and RNase H, as well as the characterization of engineered HIV-1 RTs with potential biotechnological applications.

Extraction of Cu from copper smelting through leaching using organic and inorganic lixiviants

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This study reports on the recovery of valuable metals from the copper smelting slag (CSS) collected from metal extraction plant located in, Baluchistan, Pakistan. The extraction of Cu was carried out by bath mode extraction using various acids and deep Eutectic solvents (DES). Extraction experiments were conducted using various liquid to solid ratios, temperatures and extraction times. Results show that maximum recovery of Cu and other metals is attained using H_2SO_4 and DES comprised of tetrabutylammonium chloride (CTAB) and citric acid, attaining 96 and 77 % Cu, respectively. The optimum conditions for extraction were found to be 2 h extraction time, 200 rpm stirring, 90 ^oC temperature and liquid to solid ratio of 3. The process may be upscaled by industrial scale extraction of Cu from smelting slag.

Experimental and Computational Profiling of Novel *Bis*-Schiff Base Derivatives Bearing α-Naphthalene Moiety as Potential Tyrosinase Inhibitors

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A library of novel *bis*-Schiff base derivatives **(2a-u)** of α-naphthalene moiety was successfully synthesized by four step reactions. Following structural elucidation, these products were evaluated for their in vitro tyrosinase inhibitory potential. In the series, nine derivatives **(2e, 2r, 2t, 2 g, 2 u, 2p, 2a, 2d,** and **2h)** attributed excellent inhibitory activity in the range of IC_{50} values from 2.3 ± 1.7 to 17.6 ± 0.9 μM superior to the standard drug kojic acid. Similarly, four compounds showed significant activities near to the standard while the remaining eight compounds displayed good to moderate inhibition with IC_{50} values from 29.3 ± 2.9 to 63.2 ± 1.1 μM. The molecular docking investigations for most active compounds **(2e, 2r, 2t, 2g, 2u, 2p, 2a, 2d,** and **2h)** form high stability in binding site of the tyrosinase active site, than standard kojic acid. Frontier molecular orbitals, such as HOMO and LUMO to show the charge transfer from molecule to biological medium and MEP map to show the chemically reactive zone appropriate for drug action, are calculated using TD-DFT. Besides, the drug-likeness prediction showed that these compounds showed a desirable property, such as high intestinal absorption, large volume of distribution, good BBB penetration, and low toxicity. These bis-Schiff bases have a high oral bioavailability, which can categorized as a unique drug candidate in future.

Keywords: α-Naphthalene Acetic Acid, *Bis*-Schiff Bases; Tyrosinase Inhibition; Molecular Docking

Effects of Zinc Oxide Nanoparticles coated with naturally occurring Humic Acid on Germination of Seeds

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Utilization of nanoscale materials in agribusiness are as yet in earliest stages contrasted with clinical and mechanical areas. The effect of, zinc oxide nanoparticles and humic acid (HA) coated nanoparticles were evaluated for *Brassica campestris* seed germination. A simple one-pot method was used to synthesize HA/ZnO NPs involving zinc oxide nanoparticles (ZnO) core (20-35 nm in diameter) and humic acid shell. HA/ZnO NPs were used to investigate the effect on the germination profile of *Brassica campestris*. Germination profile parameters were measured as root-shoot length, germination index, fresh and dry weight for 15 days. HA/ZnO NPs were confirmed with various physicochemical techniques such as X-ray diffraction, Fourier transform infrared (FTIR), UV-Vis spectroscopy, and scanning electron microscopy (SEM).The data confirmed the adsorption of humic acid on the surface of ZnO nanoparticles. The HA/ZnO NPs exposure significantly increased germination by 83 %, root length (60 %), shoot length (78 %), fresh weight (71.4 %) and dry weight (45.9 %).. The HA/ZnO NPs were applied as co-fertilizer to upgrade the *Brassica campestris* seed germination. Seeds may have assimilated NPs, which thus might prompt the union of specific catalysts, working with the food activation. This investigation exhibited that HA/ZnO NPs can be a capable co-compost, giving zinc and HA to seed.

Keywords: Zinc oxide nanoparticles, Humic acid, Seed germination, *Brassica campestris*, Nanoparticles.

Synthesis, Characterization, Enzyme Inhibition and Molecular Docking Studies of Benzothiazole Derivatives Bearing Alkyl Phenyl Ether Fragments

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Novel benzothiazole derivatives containing alkyl/benzyl phenyl ether fragments have been synthesized through two step reaction process. Initially, 2-hydroxybenzaldehyde was refluxed with 2-aminothiophenol in the presence of sodium metabisulfite ($Na_2S_2O_5$) in DMF solvent followed by treating it with alkyl and aromatic halides in the presence of triethylamine in dry acetone to get the product derivatives **(1-11)** in better yields. These products were characterized by means of modern spectroscopic (^{1}H, ^{13}C-NMR and HR-ESI-MS) techniques and screened for *in vitro* tyrosinase inhibitory activity. In the series, three compounds **13** (IC_{50} = 8.6 ± 0.2 µM), **3** (IC_{50} = 11.1 ± 0.5 µM), and **12** (IC_{50} = 18.2 ± 0.1 µM) showed excellent inhibition comparing with the standard kojic acid (IC_{50} = 17.8 ± 0.6 µM). Likewise, six compounds **9, 10, 11, 2, 4,** and **5** attributed significant activity ranging from IC_{50} 22.6 ± 0.8 to 29.2 ± 0.3 µM. Besides, compound **6** (IC_{50} = 40.6 ± 0.5 µM) was found least active while two compounds **7** and **8** were found inactive. The molecular docking study on molecules and their interaction with tyrosinase protein revealed a consistent pattern in the activity of kojic acid. The electronic characteristics of active derivatives **2, 3, 9-12**, and kojic acid were examined using the TD-DFT approach. The study found that the HOMO and LUMO were concentrated on the π-conjugated system of the benzothiazole rings moiety, indicating a significant delocalization of electrons. The study also found that compounds compared to kojic acid, possess chemical hardness and stability properties, with lower electrophilicity index indicating higher bioactivity and lower toxicity. The study also highlighted the importance of comprehensive ADMET profiling in early drug development to ensure safety and efficacy.

Novel Acyl Hydrazide Derivatives of Polyhydroquinoline as Potent Anti-Diabetic and Anti-Glycating Agents: Synthesis, *In Vitro* α-amylase, α-glucosidase Inhibition and Anti-glycating activity with Molecular Docking Insights

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In this study, eleven novel acyl hydrazides derivative of polyhydroquinoline were synthesized, characterized and screened for their *in vitro* anti-diabetic and anti-glycating activities. Seven compounds **2a, 2d, 2i, 2h, 2j, 2f,** and **2g** exhibited notable α-amylase inhibitory activity having IC_{50} values from 3.51 ± 2.13 to 11.92 ± 2.30 μM. Similarly, six compounds **2d, 2f, 2h, 2i, 2j,** and **2g** displayed potent α-glucosidase inhibitory activity compared to the standard acarbose. Moreover, eight derivatives **2d, 2g, 2f, 2j, 2a, 2i, 2g,** and **2e** showed excellent anti-glycating activity with IC_{50} values from 6.91 ± 2.66 to 15.80 ± 1.87 μM when compared them with the standard rutin (IC_{50} = 22.5 ± 0.90 μM). Molecular docking was carried out to predict the binding modes of all the compounds with α-amylase and α-glucosidase. The docking analysis revealed that most of the compounds established strong interactions with α-amylase and α-glucosidase. All compounds fitted well into the binding pockets of α-amylase and α-glucosidase. Among all compounds **2a** and **2f** were most potent based on docking score -8.2515 and -7.3949 against α-amylase and α-glucosidase respectively. These results hold promise for the development of novel candidates targeted at controlling postprandial glucose levels in individuals with diabetes.

Bio-Oriented Synthesis of Ibuprofen-Clubbed Novel *Bis*-Schiff Base Derivatives as Potential Hits for Malignant Glioma: *In Vitro* Anticancer Activity and *In Silico* Approach

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This research work is based on the synthesis of *bis*-Schiff base derivatives of the commercially available ibuprofen drug in outstanding yields through multistep reactions. Structures of the synthesized compounds were confirmed by the help of modern spectroscopic techniques including high-resolution electrospray ionization mass spectrometry (HR-ESI-MS), ^{1}H-NMR, and ^{13}C-NMR. The synthesized compounds were evaluated for their anticancer activity using a normal human embryonic kidney HEK-293 cell and U87-malignant glioma (ATCC-HTB-14) as a cancer cell line. All of the synthesized compounds among the series exhibited excellent to less anti-proliferative activity having IC_{50} values ranging from 5.75 ± 0.43 to 150.45 ± 0.20 *µ*M. Among them, compound **5e** (IC_{50} = 5.75 ± 0.43 *µ*M) was found as the most potent anti-proliferative agent, while **5f, 5b, 5a, 5n, 5r, 5s, 5g, 5q, 5i,** and **5j** exhibited good activity with IC_{50} values from 24.17 ± 0.46 to 43.71 ± 0.07 *µ*M. These findings suggest that these cells (HEK293) are less cytotoxic to the activities of compounds and increase the cancer cell death in brain, while the lower cytotoxicity of the potent compounds in noncancerous cells suggests that these derivatives will provide promising treatment for patients suffering from brain cancer. The results of the docking study exposed a promising affinity of the active compounds toward casein kinase-2 enzyme, which shows green signal for cancer treatment.

Thermo-Catalytic Pyrolysis of Citrus Fruit Peels over Ni-Co-Doped Molecular Sieve: Kinetic Studies

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Every day, enormous amounts of biomass are produced; a portion of this is consumed for various purposes, while the rest is burned in the open atmosphere or dumped, resulting in environmental pollution. *Citrus sinensis* (Mosami) waste, which are produced as a byproduct of eating the edible part of the citrus sinensis fruit, are also discarded as waste, contributing to environmental pollution. To mitigate this pollution and convert this waste into useful products, such as bio-oil gas and char, pyrolysis of citrus sinensis peels has been conducted without catalyst, with molecular sieve catalyst, and with Ni-Co doped molecular sieve catalyst. The catalyst and doped catalyst were characterized by EDX and XRD and were compared. GC-MS analysis of the bio-oil obtained from pyrolysis at temperatures ranging from 290 to 380 °C revealed that catalytic pyrolysis yielded more C_4-C_{26} compounds compared to non-catalytic pyrolysis that only yielded C_4-C_{24} compounds. Movreover, optimization of temperature, time and catalyst concentration were find. To determine the reaction's kinetic parameters, TGA was used to heat citrus sinensis peels at rates of 10, 20, 30, and 40 °Cmin^{-1} with and without molecular sieve 3A catalyst. TGA/DTG analysis of citrus sinensis waste revealed three stages of degradation in the temperature range of 25-600 °C, in the absence/presence of a catalyst. Average frequency factor and activation energy for non-catalyzed reaction were observed as 19.20x10^{12} min^{-1} and 118.47 kJmol^{-1} by using Kissinger method while for catalyzed reaction activation energy and frequency factor were calculated as 95.611 kJmol^{-1} and 5.75×10^{8} min^{-1}. The average activation energy was found to be lowered by catalyst from 109.05 kJ/mol to 95.611 kJ/mol. Additionaly, the thermodynamic parameters; enthalpy, entropy and Gibbs free energy were also determined.

Keywords: *Citrus sinensis* waste; Molecular sieve 3A as catalyst; Pyrolysis; Kinetics; Activation energy; Frequency factor, Thermodynamics; Ni-Co doped molecular sieve catalyst.

Bioactive steroidal alkaloids from *Haloxylon articulatum*

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Two new steroidal alkaloids have been isolated from the high polar fractions of the *Haloxylon articulatum*. The structures of the newly isolated compounds have been elucidated by the extensive use of 1D NMR and 2D NMR experiments and by the chemical analysis. *Haloxylon articulatum* belongs to the family Chenopodiaceae. This family contains 101 genera and 1220 species. 35 genera of this family are present in Pakistan. Haloxylon contain 5 species, *H. griffithii, H. recurvum, H. persicum, and H. stocksii. H. salicornicum.* Literature contains very less information for the medicinal use of *H. articulatum*. Local practitioners used this plant for the treatment of insects, snakes and scorpion bites. Previously some terpenoids have been reported from the genus Haloxylon. This prompted us to investigate the isolation of further bioactive steroidal molecules from the *H. articulatum*.

Unveiling the Potential of Bismuth Doping in Mixed Oxide of Cerium: A Key to Superior Dielectric Performance and Environmental Mitigation through Heterogeneous Photocatalysis

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Herein, we describe the synthesis of cerium molybdate ($Ce_2(MoO_4)_3$) and different compositions of Bi-doped cerium molybdate ($Ce_{2-x}Bi_x(MoO_4)_3$) where x = 0.01, 0.03, 0.05, 0.07, and 0.09, through simple co-precipitation method. The synthesized materials were optically, structurally, and morphologically characterized by various sophisticated techniques including UV-Visible, FTIR, Raman, PXRD, BET, and SEM-EDX. Upon addition of bismuth, the optical band gaps are reduced from 3.35 eV ($Ce_2(MoO_4)_3$) to 2.83 eV $Ce_{1.93}Bi_{0.07}(MoO_4)_3$. The charge storage potential and AC conductivity of the synthesized materials were investigated through dielectric studies where the dielectric constant increased by increasing dopant concentration up to 7%. At 20 Hz, $Ce_{1.93}Bi_{0.07}(MoO_4)_3$ showed a significantly greater dielectric constant (3.597×10^6) compared to undoped $Ce_2(MoO_4)_3$ (3.262×10^5). Similarly, the AC conductivity of $Ce_{1.93}Bi_{0.07}(MoO_4)_3$ increased up to 4.758 S m^{-1} compared to the undoped $Ce_2(MoO_4)_3$ (2.270 S m^{-1}) at 20 MHz. The photocatalytic efficiency was investigated against diclofenac potassium which also considerably improved by increasing the contents of bismuth. The maximum photodegradation of 87.9% was observed for $Ce_{1.93}Bi_{0.07}(MoO_4)_3$ in 180 min under UV light irradiation at optimized conditions (pH = 4, catalyst dosage = 20 mg and initial concentration of drug = 5 mg L^{-1}). The photocatalytic reaction followed pseudo-first-order kinetics with a rate constant of 0.0108 min^{-1} with stability up to five successive runs of photocatalytic activity indicating its good recyclability. These findings suggest that Bi-doped cerium molybdate could be used as a promising material for photocatalysis and energy storage devices.

Keywords: Doping; Bismuth; Heterogeneous Photocatalysis; Diclofenac degradation

Volatile constituents from leaf of *Cordia dichotoma*

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Cordia dichotoma belongs to family Boraginaceae. This tree exhibits a significant medicinal value. Its seeds demonstrate anti-inflammatory activity and fruits are astringent, expectorant, diuretic and anthelmintic. In the current study, the leaf volatile oil of this plant was extracted using hydrodistillation technique using a steam distillation assembly and a yield of 0.2% was achieved. In the next step, Gas Chromatography - Mass Spectrometry was employed for the separation and identification of a total of 21 constituents. The most abundant compounds were phytol, palmtic acid, *p*-vinylguaiacol, trans-phyt-2-ene and cinnamaldehyde, respectively. Most of the identified compounds are bioactive in nature that proves the medicinal importance of this plant.

Keywords: Cordia dichotoma, Boraginaceae, volatile composition, phytol, palmitic acid

Poly-hydroxyl butanolides from *Calligonum pollygonoides*

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Calligonuolide A and B, two new new butanolides have been isolated from the whole plant of *Calligonum polygonoides*. Their structures have been elucidated through spectral studies. They showed moderate inhibitory potential against the enzyme lipoxygenase. The genus *Calligonum* belongs to the family Polygonaceae which comprises 80 species distributed throughout Western Asia, Southern Europe and Northern Africa. In Pakistan this genus is represented by only one species namely *C. polygonoides*. It is a slow growing almost leafless shrub. A decoction of the roots mixed with catechu is used as gargle for sore gums, while the shoot juice is applied to the eyes as an antidote to scorpion sting. The latex is used to induce abortion, to cure bites of rabid dogs and for treating eczema. The flowers possess digestive ad tonic properties and are useful in cough, cold, and asthma.

Phytochemical Profiling and Molecular Docking: *Citrus sinensis* as a Source of Neuroprotective Agents

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Neurotoxicity is the rising concern by the prevalent use of cosmetic products. Owing to the negative consequences of prescribed drugs for treatment, present research explored the neuroprotective efficacy of flavonoids of *Citrus sinensis* and their ability to mitigate neurotoxicity using In silico techniques, molecular docking studies against neurotoxic protein targets, ADMET profiling and phytochemical identification via Liquid chromatography mass spectrometry (LCMS/MS). The study also used the PASS prediction and the neurotoxic proteins' (4EY5 and 6I0C) high docking score to project the unusual biological activity of nervous systems in treating illnesses. Resveratrol was observed to be the major neuroprotective phytocompound which have strong binding (-11.8445 kcal/mol) to 4EY5 with participating amino acids of GLY A:121, TYR A:124, SER A:203, TYR. Moreover, resveratrol with strong binding to 6I0C found to be the optimal compound with participating amino acids of (TYR A:332, PRO A:285, PHE A:329, ALA A:328). MDS results showed that the hydrophobic interactions are significantly high with the specified amino acid residues in protein 4EY5. These amino acid residues were LEU-76, TRP-86, TRY-124, TRP-286, PHE-297, TYR-337, PHE-338, HIS-447. The protein 6I0C projects the major protein-ligand interactions with hydrogen bonds. The hydrogen bonds interacts with ILE-14, SER-15, GLU-34, ARG-42, GLY-434, the residues of specified amino acids. The current study findings suggested that the flavonoids of Citrus sinensis can be employed in neurodegenerative disorders as neuroprotective agents.

Keywords: *Citrus sinensis*; Neurotoxicity-inhibition; In-silico; ADME; Molecular Docking; MDS.

Exploring cucumber-derived phytochemicals for the Treatment of Periorbital Hyperpigmentation through *In-vitro* and *In Silico* analysis

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Periorbital hyperpigmentation results from increased melanin deposition and can be influenced by genetics, sun exposure, fatigue, hormonal changes, or certain medical conditions. This study aims to fill the gap in understanding the biochemical basis of periorbital hyperpigmentation and investigates the potential of phytochemicals in cucumber to combat this condition through in vitro and in silico studies. The liquid chromatography mass spectrometry (LCMS) was employed to identify active phytochemicals involved in inhibiting periorbital hyperpigmentation, while the molecular docking was used to determine the ligand and binding sites of target protein Tyrosinase (PDB ID:5M8R). In vitro analysis explored the Tyrosinase inhibition potential of these phytochemicals. The ADME (absorption, distribution, metabolism and excretion) analysis revealed that the average bioavailability score of cucumber phytochemicals exceed the ideal threshold of ≥0.55. Molecular docking showed that eicosenoic acid achieved the highest docking score of -11.728 with Tyrosinase. MDS analysis over 100ns confirmed the stability of eicosenoic acid within the Tyrosinase binding sites, suggesting that its effectiveness against periorbital hyperpigmentation by inhibiting the melanin producing enzyme Tyrosinase. Additional results showed that other phytochemicals such as caffeic acid and ferulic acid, also exhibited significant binding affinities, with docking scores of -9.45 and -9.87 respectively. These compounds were assessed for the ability to inhibit Tyrosinase through *In vitro* assays. Eicosenoic acid showed the strongest Tyrosinase inhibition with an IC50 value of 2.1µM, indicating a potent inhibitory effect on melanin synthesis. These findings suggest that various compounds in cucumber may contribute to reducing periorbital hyperpigmentation through Tyrosinase inhibition.

Keywords: Periorbital hyperpigmentation; Melanine; Cucumbe; In silico studies; LCM; Tyrosinase inhibition; Molecular Docking

Pollutants Concentration during the Construction and Operation Stages of a Long Tunnel: A Case Study of Lowari Tunnel, (Dir-Chitral), Khyber Pakhtunkhwa, Pakistan

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Long tunnels with significant overburden, changeable geological conditions, a steep gradi- ent, water infiltration, and heavy traffic flow are susceptible to environmental concerns during both construction and operation. The availability of fresh air and visibility is the most important necessity in excavation for tunnel workers inside the tunnel during the construction phase, as well as those crossing the tunnel during operation. Lowari Tunnel's tunnel air pollutants were researched. Carbon monoxide (CO), carbon dioxide (CO_2), oxygen (O_2), hydrogen sulfide (H_2S), sulfur dioxide (SO_2), nitrogen oxide (NO), ammonia (NH_3), nitrogen dioxide (NO_2), PM1, PM2.5, PM10, air velocity, dust morphological and particle size distribution analysis are among the parameters under consideration. The findings provide evidence for the development of tunnel air quality.

Keywords: road tunnel; construction stage; operation stage; gases concentration; particulate matter; environmental monitoring and engineering.

Microwave Assisted Green Synthesis of Zinc Oxide Nanoparticles Using Paneer dodi (*Wathania Coagulans)* Fruit Extract, Antioxidant Potential of Extract and their Photocatalytic Activity for Dye Degradation

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In the current study, zinc oxide nanoparticles (ZnO NPs) were fabricated and characterized utilizing *Wathania coagulans* fruit extract. The fabricated ZnO NPs from *W. coagulans* extract was characterized employing various techniques such as UV-visible spectroscopy (UV-vis), X-ray diffraction (XRD), Scanning electron microscope (SEM), Fourier transform infrared (FTIR). The prominent peak at 365 nm was measured for zinc oxide NPs. The SEM analysis showed the NPs was extremly spherical shape. The XRD peaks confirmed the crystalline form of ZnO NPs. Then ZnO NPs was analyzed by FTIR for ZnO functional group near 500 cm^{-1}. The *W. coagulans* extract was examined for their antioxidant properties having exhibited high total phenolic and total flavonoid contents and also exhibited moderate free radical scavenging activity. The fabricated ZnO NPs was investigated for their photocatalytic activity (PCA). The photocatalytic activity (PCA) was assessed against the dye degradation and we found to be 90 % degradation within 240 min. So, the green synthesized nanoparticles have demonstrated prominent bioactivity and photocatalytic activity, the fabrication of these NPs employing *W. coagulans* fruit extracts is advocated for various applications.

Keywords: ZnO Nanoparticles; Green synthesis; Antioxidant; Photocatalytic activity

Curcumin's molecular interactions: an exploration of its potential against skin cancer targets using *in-vitro* and *in-silico* techniques

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Melanoma is the most invasive skin cancer with the highest risk of death. The methanol extracts of *Curcuma longa* were thoroughly evaluated as potential sources of anti-melanoma chemicals. The current study focuses on identifying the phytochemicals, and absorption, distribution, metabolism, excretion and toxicity analysis, molecular docking to evaluate binding affinities against skin cancer relevant protein and molecular dynamic simulations to investigate the interactions and stability of compound with proteins relevant to skin cancer. LCMS analysis demonstrate the presence of sesquiterpenes and polyphenols. Additionally, B16-F10 and SK-MEL-28 skin cancer cell lines were used in vitro anti melanoma investigations, with IC50 values of 73.80618 µg/ml and 36.19 µg/ml, respectively. The topical candidates identified from LCMS with a focus on ADMET and lower LogKP values, are permeating the dermis. Toxicity profiling demonstrates the safety of using phytochemicals as medications without any fatal side effects. For the proteins of skin cancer (crystal structure of an anti-ssDNA antigen-binding fragment (Fab) and Serine/threonine-protein kinas MRCK beta), distinct biological activity and a strong docking score were predicted. The phytocompound with the highest binding energy for human skin cancer is Ar-turmerone (-12.5204 kcal/mol) to 1P7K, whereas the best chemical was Beta-Turmerone (-12.0979 kcal/mol) to 5OTE. MD simulation of Ar-turmerone against 1P7K and beta-Turmerone against 5OTE over 100ns demonstrated significant anti-skin cancer potential. According to our findings, plants can serve as a source of natural components that can be significantly used to make a new therapeutic agents against skin cancer.

Keywords: *Curcuma longa;* Anti-melanoma; MTT assay; In-silico; ADME

Exploring the XO Inhibitory Potential of Coconut-Derived Fatty Acids: A Comprehensive *in Silico* Study for Hyperuricemia Management

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Hyperuricemia is characterized by overproduction or under-excretion of uric acid in the blood. This work aims to deliver an inclusive overview of the Xanthine oxidase (XO) inhibitory activity of fatty acids derived from *Cocos nucifera* to combat hyperuricemia through In Silico studies. It also aims to fill the gap in understanding the biochemical basis of XO-mediated diseases and elucidate the potential mechanisms underlying the inhibitory activity of coconut-derived fatty acids against xanthine oxidase. Our study involves absorption, distribution, metabolism, excretion, and toxicity (ADMET), gas chromatography-mass spectrometry (GC-MS), and Molecular Dynamic Simulation for the identification of inhibitory compounds, while in Silico pharmacokinetics and molecular docking studies were performed to gain insights into the potential interactions between these compounds and xanthine oxidase. Results from ADMET showed elevated GI absorption of phytochemicals in *Cocos nucifera* making it an effective treatment for hyperuricemia. Phytochemicals with the highest binding energies for hyperuricemia are mystiric acid (-11.7878), oleic acid (-10.0252), Palmitic acid (-10.5282), and lauric acid (-10.6175). Amino acids in stable binding are, ILE:750, TYR:1824, and THR:1010, ARG:880, for caprylic acid and lauric acid respectively. The highest binding energies of phytochemicals were subjected to MDS to determine protein-ligand interaction. According to our findings, *Cocos nucifera* can serve as a source of anti-hyperuricemia drug.

Keywords: Hyperuricemia; *Cocos nucifera*; xanthine-oxidase; molecular docking; GI absorption.

Synthesis and Applications of N-doped ZnO nanoparticles Photo-catalyst

Muhammad Salman and Umar Farooq

The study focused on the synthesis of Nitrogen doped ZnO nano particles and its applications for the removal of Brilliant green dye in the presence of white light (LED source). ZnO nano particels were synthesized by using *Juglans regia* plant's concentrate and then nitrogen doping was performed using urea. The prepared material was characterized by FTIR and employed for the degradation of Brilliant green dye from simulated solution. 89-91% degradation was observed. Band gap energy was also calculated.

Bioactivity-Guided Isolation of Polyphenols from *Citrullus colocynthis* for Antihypertensive Effect in Spontaneous Hypertensive Rat Model

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The aim of the present study was to investigate the antihypertensive effect of polyphenol-rich Citrullus colocynthis (CC) fractions against spontaneous hypertensive rats (SHR) model. Crude CC extract was fractionated in hexane, chloroform, ethyl acetate, butanol and aqueous ethanol to get hexane fraction (HEF), chloroform fraction (CHF), ethyl acetate fraction (EAF), butanol fraction (BUF) and aqueous ethanol fraction (AEF), respectively. The AEF represented the maximum yield (58.6 g/100g) followed by BUF (16.5 g/100g), HEF (3.7 g/100g), EAF (2.9 g/100g) and CHF (2.3 g/100g). The EAF contained the highest total phenolic contents (289.4 mg/g), total flavonoid contents (7.60 mg/g) and flanonol contents (35.7 mg/g). EAF showed highest DPPH radical scavenging activity (SC50, 6.2 μg/mL) followed by CHF (SC50, 17.3 μg/mL), BUF (SC50, 22.4 μg/mL), AEF (SC, 53.7 μg/mL) and HEF (SC50, 115.9 μg/mL). Best reducing potential was also observed from EAF. The RP-HPLC analysis of CC fraction revealed the presence of ferulic acid, vanillic acid, p-coumeric acid, gallic acid, p-hydroxy benzoic acid and chlorogenic acid, catechin, rutin, quercetin, myricetin and kaempferol. CC fraction dose of 250 and 500 mg kg-1 body weight were given to male SHR and WKY rats daily for 21 days through oral gavage. Rats body weight, heart rate, blood pressure were monitored twice a week. The oxidative status of the animals was determined by conducting a series of tests from collected plasma including measurements of malondialdehyde (MDA), superoxide dismutase (SOD), reduced glutathione (GSH), nitric oxide (NO) and total antioxidant capacity (TAC) levels. Best antihypertensive effect was observed in higher doze (EA-500) group in term of decrease in blood pressures. Surgery was performed at the end of the study and blood pressure, pulse wave velocity (PWV) and echocardiogram (ECG) were recorded. It was concluded that EAF of CC possessed significant antihypertensive and antioxidant activity in the SHR group.

Keywords: SOD; Quercetin; pulse wave velocity; GSH

Thermodynamics of Malachite Green Adsorption from Aqueous Media using Beans Biomass Composites

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The toxicity of water caused by dyes is significantly more dangerous for human health as well as the environment. Each year, almost 70 % of people become unwell and 60,000 people die as a result of diseases caused by water pollution. Various synthetic dyes are undervalued as environmental hazards; they are currently categorised as micropollutants in aquatic ecosystems due to their low concentrations (mg/L to g/L). Adsorption is the most effective method for the removal of dyes from wastewater. Hence, several organic and inorganic substances have been used as an adsorbents but biomasses possess promising characteristics for remediation of the contaminated water. Biomass-based composites were employed as an adsorbent since they have improved adsorptive characteristics. The surface morphologies, functional groups and crystalline structure were studied using SEM, FT-IR, and XRD, respectively. The efficacy of the biocomposites in removing malachite green (MG) was encouraging. The magnetic composite showed the best performance over all others in terms of efficiency at pH 8, 0.05 g of adsorbent, 90 min of contact duration, and 5 mg/L initial concentration at 30 °C. The Freundlich isotherm model (R^2 = 0.993) provided the best description of this adsorption process, and the dynamics analysis revealed that the Pseudo-2nd-order model (R^2 = 0.996) offered the best fitness to MG adsorption. According to thermodynamic analysis, the adsorption process was exothermic, chemisorption, and spontaneous. According to desorption experiments, substantial levels of dye desorption were caused by modest concentrations of eluting reagents. The manufactured composites demonstrated a high affinity for dye adsorption in the context of the present analysis, and this innovative class of adsorbent may be employed to create new adsorbents for environmental applications.

Keywords: Adsorption, Beans Biomass, Magnetic composite, Malachite Green, Thermodynamics

Biogenic Silver Nanoparticles from *Agastache rugosa* Functionalized with Polydopamine and Conjugated with Ceftazidime: Enhanced Antibacterial and Antibiofilm Activity Supported by Molecular Docking Studies

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Silver nanoparticles (AgNPs) have garnered significant attention for their potent antibacterial properties, yet research on sustainable synthesis and alternative antimicrobial strategies remains limited. This study presents a comparative analysis of the antibacterial potential of AgNPs synthesized from *Agastache rugosa* leaves extract, and their surface modifications with poly(vinylpyrrolidone) (PVP), and polydopamine (PDA) and conjugation with ceftazidime. Additionally, it examines the conjugation of PDA-coated AgNPs with ceftazidime to enhance antibacterial activity against *P. aeruginosa*. The study also explores the active compounds in Agastache rugosa through molecular docking studies with bacterial proteins. AgNPs were synthesized using a rapid PDA deposition process, forming PDA@AgNPs nanocomposites. These were further conjugated with ceftazidime using Sulfo-NHS and EDC to create PDA@AgNPs-Cfz. Characterization was performed using UV-Vis spectroscopy, FT-IR, and TEM. The TEM analysis confirmed that the sizes of AgNPs, PVP-AgNPs, and PDA@AgNPs were 18.52, 23.88, and 25.3 nm, respectively. The PDA@AgNPs-Cfz nanocomposite showed superior antibacterial efficacy against P. aeruginosa, with improved biofilm inhibition and MIC and MBC compared to ceftazidime alone and AgNPs, and reduced toxicity compared to AgNPs alone. Molecular docking studies of *Agastache rugosa* compounds with bacterial proteins provided valuable insights into their potential antibacterial activity. This study highlights a synergistic approach involving ceftazidime and PDA@AgNPs, offering a novel perspective on bacterial infection treatment. It emphasizes sustainable synthesis methods and alternative antimicrobial strategies. The findings suggest that PDA@AgNPs combined with ceftazidime could effectively combat antibiotic-resistant bacteria, while molecular docking studies enhance understanding of the antibacterial mechanisms of Agastache rugosa compounds.

Keywords: Silver nanocomposite, Ceftazidime conjugation, Biofilm inhibition, Molecular docking.

Mechanistic insights into eco-friendly synthesized AgNPs for biological applications against antibiotic-resistant bacteria: An *in silico* approach and toxicity evaluation using *Artemia salina*

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Antibiotic resistance poses a significant public health threat, particularly with biofilm-forming pathogens like *Pseudomonas aeruginosa*, known for its multidrug resistance (MDR) and ability to form persistent biofilms. The failure of conventional antibiotics has led to alternative approaches, including nanotechnology, to combat bacterial infections. In this study, silver nanoparticles (AgNPs) were synthesized using *Rosmarinus officinalis* (rosemary) extract, and their antibacterial and antibiofilm activities against P. aeruginosa were evaluated. Rosemary-mediated AgNPs (Rm-AgNPs) were characterized through UV-Vis spectroscopy, TEM, DLS, FTIR, and SEM-EDX analysis, confirming their successful synthesis, triangular morphology, and stability. The antibacterial mechanism of Rm-AgNPs was investigated, showing significant membrane disruption, reactive oxygen species (ROS) generation, protein/DNA leakage, and genomic DNA damage in *P. aeruginosa*. Rm-AgNPs exhibited strong antibacterial activity, with a minimal inhibitory concentration (MIC) of 32.5 μg/mL and pronounced antibiofilm effects, inhibiting biofilm formation by up to 65.68% at 2xMIC. Further analysis revealed that Rm-AgNPs induce oxidative stress, leading to glutathione depletion and increased ROS levels, contributing to bacterial cell death. Molecular docking studies explored interactions between rosemary phytochemicals and key proteins involved in biofilm formation and quorum sensing in *P. aeruginosa*. Compounds like Alnuside A and Umbelliferone exhibited strong binding affinities, suggesting their potential as quorum-sensing inhibitors. Toxicity studies using brine shrimp *(Artemia salina)* revealed that Rm-AgNPs were less toxic than $AgNO_3$, with an LC_{50} value of 202.55 μg/mL. This study highlights the potential of eco-friendly synthesized Rm-AgNPs as effective antibacterial and antibiofilm agents against drug-resistant pathogens, offering promising alternatives to conventional antibiotics.

Keywords: Silver nanoparticles, Eco-friendly synthesis, Anti Biofilm inhibition, Molecular docking.

Exploring Novel *β*-Indolyl Ketones as Potent Aromatase Inhibitors through *In-Vitro* and *In-silico* Studies: Unraveling Heme-ligand Interactions by MD Simulation, and MMPBSA Analysis

Shanza Munir

A series of enantioenriched *β*-indolyl ketones as aromatase inhibitors (AI) is synthesized through the Michael-type Friedel-Crafts alkylation of indole. For this purpose, a highly efficient bi-functionalized amino catalyst is developed to access structurally diverse *β*-indolyl ketones in high yields (up to 91%) and excellent enantioselectivity (er up to 98:2). Aromatase inhibitory potential of the synthesized *β*-indolyl ketones demonstrated promising inhibition activity, where ortho-substituted analogs (**3c** and **3e**) were found most active (IC_{50}= 0.68 and 0.90 μM). Molecular docking studies were performed to understand the mode of interactions, where the synthesized compounds demonstrate favorable binding interactions with the estrogens controlling enzyme CYP19A1 (3EQM) and metabolizing enzyme CYP3A4 (5VCC). The docking results and MD simulation analysis revealed the essentiality of developing interaction with the Heme group to build a stable protein-ligand complex. Compound **3**, inside the Heme-binding pocket of 3EQM, exhibited an average root-mean-square deviation (RMSD) of 0.35 nm, and binding energy in the range of -190 to -227.0 KJ/mol through the g_mmpbsa analysis, authenticated the stability of the **3c-3EQM** complex. The bioavailability and pharmacokinetic parameters supported the suitability of these indole derivatives to develop potent inhibitors for estrogen-dependent breast cancer.

Plant-based Metal Nanocomposites as Potent Leishmanicidal and anti-microbial agents

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Successful fabrication of MgO-ZnO bimetallic nanoparticles was achieved, utilizing the oily extract of *Curcuma zedoaria*. Varying metal ratios were used to fabricate nanocomposites with metals in 1:1, 1:2, and 2:1 ratios. The composites were characterized with the help of X-ray diffraction, infra-red and UV/visible spectroscopy, scanning electron microscopy, and thermogravimetric studies, exhibiting a thermally stable and crystalline nature, with crystallite sizes ranging between 4.01-8.12 nm. The anti-bacterial potential of the composites were found to be higher as compared to their precursor extract. One of the composites, also exhibited significant anti-fungal activity against *Fusarium graminearum*. The composites also showed good Leishmanicidal activity, with IC_{50} of 46.27 ± 2.73, 50.47 ± 3.589, and 72.11 ± 3.14 μg/mL, for Mg_1Zn_1, Mg_1Zn_2, and Mg_2Zn_1, respectively.

Keywords: Anti-microbial, Bimetallic nanoparticles, *Curcuma zedoaria*, *Leishmania tropica*.

Synthesis and Potential Applications of New Functionalized Task Specific Ionic Liquids (TSILs)

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The current work explains the synthesis of new functionalized azolium-based ionic liquids (ILs) from easily accessible alcohols. An exhaustive characterization was performed using state-of-the art techniques, such as MS, IR and NMR spectroscopy. Thermal properties of the synthesized ionic liquids were studied by TGA and DSC analyses. Moreover, computational studies were employed to explore the physicochemical properties of the prepared ionic liquids. Applications of the newly synthesized ILs were demonstrated as chiral shift agents and as bifunctional organocatalyst.

Keywords: Azolium-based ionic liquids (ILs), chiral shift agents, organocatalyst.

Deciphering the Molecular Mechanisms of 7-Desacetyl-7-Benzoylazadiradione: Examining its Effect on Target Gene Expression as a Potential Scabicide Agent - An Integrated Analysis Combining *In Vitro* and *In Silico* Approaches

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Acute post-streptococcal glomerulonephritis is the major consequence of negligent diagnosis and treatment of *Sarcoptes scabiei*. The study evaluated the acaricidal potential of bioactive components of *Azadirachta indica* against mite mortality and scabies using both In vitro and In silico methodologies. Mites were stimulated with 10% ivermectin (positive control) at four concentrations (25-100 mg/ml) at different intervals. In silico analysis includes prediction of target, toxicity evaluation, biological activity, protein structure, and gene expression. LCMS was used for the analysis of phytoconstituents and Molecular docking for the characterization of bioactive components. AdmetSAR-2.0 web server was used to assess the site of metabolism, biodegradation, and in silico toxicity evaluation in rat and fish model. In-vitro analysis suggests that *Azadirachta indica* has a dose-dependent effect on *Sarcoptes scabiei* at different time intervals. With a docking score of −12.324 kcal/mol, 7-desacetyl-7-benzoylazadiradione showed significant inhibitory interactions with the glutathione transferase protein of *S.scabiei*, outperforming permethrin. Arginine: 58 and Serine: 56 amino acids were implicated in the production of hydrogen bonds. Even though the trpB, trpA, and trpD genes had tighter protein-protein interactions. All of the target genes IDs with the highest probability of corresponding to 7-desacetyl-7-benzoylazadiradione were used for a gene expression network. With a high hyper-geometric p-value, the total interactions between transcription factors, kinases, and intermediate proteins are observed. It was concluded that *Azadirachta indica* can be used as a natural substitute for managing mite infestations and offered understanding into the mechanisms by which its phytochemicals inhibit these infections

Keywords: *Sarcoptes scabie*; acaricidal; *Azadirachta indica*; In silico analysis; S. scabiei glutathione transferase

Modulation of the SIRT1 Gene by Phytoconstituents of *Aloe barbadensis*: A Key Intermediate in the Aging Process"

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Skin aging is one of the most obvious signs of human aging. Peeling and itching are common side effects of skin anti-aging products available in the market. The purpose of this study was to assess the skin permeability, antioxidant, anti-inflammatory, and anti-aging effects of *Aloe barbadensis* phytoconstituents using computational techniques. Molecular docking was used to explain the energy required to pulling apart Ligand-Receptor. Phytol, Lupeol, Lophenol, Sitosterol, Eicosane, and Cycloartenol were found to be used as skin permeant product at a skin permeability threshold of −5.0 cm/s. Molecular target prediction found tyrosinase, 11-beta-hydroxysteroid dehydrogenase 1, androgen receptor and cyclo-oxygenase-1 as potential targets. Lupeol with LogKP value of -1.9 with docking score (-14.1523 kcal/mol) and Lophenol with skin permeability of -2.55 with docking score (-13.3135 kcal/mol) found to have strong binding effects with target protein of cyclooxygenase, but Cycloartenol (-10.2971 kcal/mol) and Lupeol (-10.988 kcal/mol) showed high antioxidant activity. Furthermore, the SIRT1 gene was found to be an important intermediate in the aging process, tying *Aloe barbadensis*' bioactive compounds for anti-aging potential. The study finds that dermatologists can use the *Aloe barbadensis* to improve dermal and epidermal histology, lower inflammatory indicators, and ameliorate wrinkle formation.

Keywords: In-silico; skin permeation; pharmacokinetics; molecular docking; protein-protein interaction.


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