Book of Abstracts

International Conference on

Innovation in Chemistry and Physics (ICP-2022)

Organized by

University of Education, Faisalabad Campus

March 14-15, 2022

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1	Mr. Ahmad Azam	Convener
2	Mr. Naukhaiz Chaudhary	Member
	Mr. Farhan Mahuddin	Member

Conference Program ICP-2022
Day-I
14th March, 2022.

Timeline	
Registration Library Entrance, UE Faisalabad Campus. 8:00 am PST	
Inauguration Main Hall, UE Faisalabad Campus. 8:30-09:30 am PST	
08:30-09:30 am	Recitation from the Holy Quran by Mr. Hafiz Muhammad Mazhar Iqbal Naat-e-Rasool e Maqbool by Ms Fareeha Ashraf Welcome Note by Prof. Dr. Muhammad Abid Rashid. Remarks by Principal UE Vehari Campus Prof. Dr. Sheikh Israr Ahmad Remarks by Distinguished Guest Prof. Dr. Robina Farooq Vice Chancellor GCWUF Word of wisdom by Patron in Chief, Prof. Dr. Talat Naseer Pasha (SI) Vice Chancellor University of Education, Lahore Remarks by Chief Guests Prof. Dr. Khalid M. Khan (SI, TI). President Chemical Society of Pakistan. HEJ, Karachi Remarks by International Chair, Prof. Dr. David Morales-Morales, Universidad Nacional Autonoma, Mexico. Distribution of Shields/Certificates
Plenary Lectures Main Hall, UE Faisalabad Campus. 09:30-11:15 am PST Session Convener: Dr. Muhammad Yaseen and Dr. Nosheen Rashid, University of Education, Faisalabad.	
09:30-10:05 am	Prof. Dr. David Morales-Morales, Universidad Nacional Autonoma, Mexico.
10:05-10:40 am	Prof. Dr. Khalid M. Khan (SI, TI). President Chemical Society of Pakistan. HEJ, Karachi.

10:40-11:15 am	Prof. Dr. Muhammad Hassan Sayyad, Ghulam Ishaq Khan Institute of Engineering Science and Technology, Swabi
Tea Break/Poster Session Library ground/Library Greens, UE Faisalabad Campus. 11:15-11:45 am PST	
Keynote Lectures Main Hall, UE Faisalabad Campus 11:45-02:15 pm PST Chair: Prof. Dr. Khalid M. Khan (SI, TI). President Chemical Society of Pakistan. HEJ, Karachi. Co-Chair: Dr. Imran, Department of Pharmacology, Faculty of Pharmacy, BZU, Multan Session Convener: Dr. Muhammad Yaseen and Dr. Nosheen Rashid, University of Education, Faisalabad Campus.	
11:45-12:15 pm	Prof. Dr. Syed Ghulam Musharraf, HEJ, University of Karachi.
12:15-12:45 pm	Prof. Dr. Bilal Masud, Director of Center for High Energy Physics, University of the Punjab, Lahore.
12:45-01:15 pm	Prof. Dr. Zaheer Ul Haq Qasmi, HEJ, University of Karachi.
01:15-01:45 pm	Dr. Faisal Akram, Center for High Energy Physics, University of the Punjab, Lahore.
01:45-02:15 pm	Dr. Yasir Jamil, Chairman, University of Agriculture, Faisalabad.
Lunch and Prayer Break Library Ground, UE Faisalabad Campus. 02:15-03:00 pm PST	
Parallel Session I: Online Room A29, UE Faisalabad Campus. 03:00-06:00 pm PST Session Convener: Dr Ishrat Asghar, Dr. Zahid Farooq, Dr. Munawar Iqbal, University of Education, Faisalabad Campus	
03:00-03:30 pm PST	Prof. Dr. Arif Demir, Laser Physics Engineering, Istanbul Turkey.
03:30-04:00 pm PST	Dr. Dursan Kisa, Kutlinbey Campus, Bartin University, Turkey.
04:00-04:30 pm PST	Dr. Ghulam Ali, US-Pakistan Center for Advanced Studies in Energy, NUST.
04:30-05:00 pm PST	Dr. Ibrahim Fazil Segul, Department of Chemistry, faculty of Science, Technical University, Kocaeli, Turkey.

05:00-05:30 pm PST	Dr. Nazir Tahir, University of Windsor, Windsor, Canada.
05:30-06:00 pm PST	Dr. Simon Rondeau-Gagne, University of Windsor, Canada.

Parallel Session II: Organic & Biochemistry

Main Hall, UE Faisalabad Campus.
03:00-04:30 pm PST
Chair: Prof. Dr. Syed Ghulam Musharraf, HEJ, University of Karachi.
Co-Chair: Prof. Dr. Zaheer Ul Haq Qasmi, HEJ, University of Karachi.
Session Convener: Dr. Muhammad Yaseen, Dr. Aeysha Sultan, University of Education, Faisalabad Campus.

Time	Topic	Presenter	Affiliation
03:00-03:15 pm PST	Labeling of linzolid with Technetium-99m and its biodistribution in Swiss Albino mice	Dr. Tanveer Hussain Bokhari	Department of Chemistry, Government College University, Faisalabad
03:15-03:30 pm PST	Biotransformation of organic wastes into value-added products: recent developments and challenges	Dr. Tahir Mehmood	Centre for Applied Molecular Biology (CAMB), University of the Punjab, Lahore
03:30-03:45 pm PST	Synthesis and antioxidant screening of Novel indole amines	Dr. Syeda Laila Rubab	Department of Chemistry, University of Education (Lahore), Jauharabad campus
03:45-04:00 pm PST	Optimization and impact of different extraction parameters to extract phytochemicals from dried Phlomis stewartii leave's using Response surface methodology	Mamoon Ur Rasheed	Department of Chemistry, Government College University, Faisalabad
04:00-04:10 pm PST	Improved bioavailability of Ebastine through development of transfersomal oral films	Nayyer Islam	Department of Pharmaceutics, Government College University, Faisalabad
04:10-04:20 pm PST	Designed synthesis of thiobarbituric acid hybrid structures as potent urease inhibitors	Dr. Zulfiqar Ali Khan	Department of Chemistry, Government College University, Faisalabad
04:20-04:30 pm PST	Bio-surfactant is a potent tool for the Bioremediation	Dr. Muhammad Yameen	Department of Biochemistry,

	of heavy metals and organic compound in contaminated soil and water		Government College University, Faisalabad
04:30-04:45 pm PST	Single Nucleotide Polymorphism analysis of APOA5 Gene In HypertriglyceridemiC Patients	Dr. Nosheen Aslam	Department of Biochemistry, Government College University, Faisalabad Pakistan

Parallel Session III: Inorganic, Analytical & Physical Chemistry

Room A28, UE Faisalabad Campus.
03:00-04:30 pm PST
Chair: Prof. Dr. Haq Nawaz Bhatti, Department of Chemistry, UAF.
Co-Chair: Dr. Haq Nawaz, Department of Chemistry, UAF.
Session Convener: Dr Naveed Ahmad, Dr. Hafiz M. Abdul Qayyum, University of Education, Faisalabad Campus.

Time	**Topic**	**Presenter**	**Affiliation**
03:00-03:15 pm PST	Micellar Enhanced Flocculation for removal of pollutants from synthetic waste water	Dr. Muhammad Usman **(Invited Speaker)**	Department of Chemistry, Government College University, Faisalabad
03:15-03:30 pm PST	Development of Bi_2O_3-ZnO heterostructure for enhanced photodegradation of Rhodamine B and reactive yellow dyes	Dr. Muhammad Saeed	Department of Chemistry, Government College University, Faisalabad
03:30-03:40 pm PST	Improvement of activity, thermo-stability and fruit juice clarification characteristics of fungal exo-polygalacturonase	Dr. Faiza Amin	Department of Chemistry, Government College Women University Faisalabad, Pakistan
03:40-03:50 pm PST	Stoichiometric architectural impact on thermo-mechanical and morphological behavior of segmented Polyurethane elastomers	Dr. Nadia Akram	Department of Chemistry, Government College University, Faisalabad
03:50-04:00 pm PST	Optimum Conditions for the removal of Rhodamine B from aqueous system by micellar enhanced ultrafiltration.	Amnah Yusaf	Department of Chemistry, Government College University Faisalabad Pakistan

04:00-04:10 pm PST	Investigation of Photo-esterification capability of RGO/$BiVO_4$ for the production of Biodiesel from soapnut oil and its computational study.	Dr. Naila Ghani	Department of Chemistry, University of Agriculture, Faisalabad.
04:10-04:20 pm PST	Patterns of essential/toxic metals distribution in blood of diabetes mellitus patients in comparison with healthy donors.	Dr Hafiz Muhammad Abdul Qayyum	Department of Chemistry, University of Education, Lahore, Faisalabad campus.
04:20-04:30 pm PST	Investigation of Cu-doped zinc oxide Zn1-xCuxO (x = 0.01, 0.02, 0.03, 0.04, 0.05) based nanostructures for the elimination of Methylene Blue dye pollutant under sunlight	Umair Khalid	Department of Physics, University of Management and technology Lahore Pakistan

Parallel Session IV: Theoretical & Applied Physics

Video Conference Room, UE Faisalabad Campus.

03:00-04:30 pm PST

Chair: Prof. Dr. Afaq Ahmad, Center of Excellence in Solid State Physics, University of the Punjab, Lahore

Co-Chair: Dr. Umber Sheikh, Department of Mathematics, UE Faisalabad.

Session Convener: Ms Ambreen Aslam, Dr Ishrat Asghar, University of Education, Faisalabad Campus.

Time	Topic	Presenter	Affiliation
03:00-03:15 pm PST	Recent R&D activities at Atomic and Laser Physics, NCP Islamabad	Dr. Rizwan Ahmad	Atomic and Laser Physics, National Centre for Physics (NCP), Islamabad.
03:15-03:30 pm PST	Assessment of Soft Tissue Substitutes for megavoltage photon beams	Unaiza Kashif	RIUF, Pakistan, UE Faisalabad; Department of Physics, university of Education Lahore, Faisalabad Campus.
03:30-03:45 pm PST	Photocatalytic degradation of Methyl Green dye mediated by pure and Mn doped Zinc Oxide nanoflakes under solar light irradiation	Adeena Fatima	Department of Physics, University of Management and Technology, Lahore
03:45-04:00 pm PST	On Dynamics of Anisotropic Compact Stars in Rainbow	Dr. Umber Sheikh	Department of Mathematics, UE

	Gravity		Faisalabad.
04:00-04:15 pm PST	Estimation of ABC and GA indices of Fullerenes.	Qurrat-ul-Ain	National Textile University, Faisalabad.
04:15-04:30 pm PST	Synthesis, characterization, and antimicrobial application of $Mg_xZn_{1-x}Fe_2O_4$	Dr. G.R. Sani	University of Agriculture, Faisalabad
Parallel Session V: Material Sciences Room A32, UE Faisalabad Campus. 03:00-04:30 pm PST Chair: Dr. Faisal Akram, Center for High Energy Physics, University of the Punjab, Lahore. Co-Chair: Dr. Imran Din, School of Chemistry, University of the Punjab, Lahore Session Convener: Dr G.M. Mustafa, Dr. Zahid Farooq, Dr. Munawar Iqbal, University of Education, Faisalabad Campus.			
Time	**Topic**	**Presenter**	**Affiliation**
03:00-03:15 pm PST	Green synthesis of stable and monodisperse CuO nanoparticles using punica granatum extract as a reducing agent	Dr. Imran Din **(Invited Speaker)**	School of Chemistry, University of the Punjab, Lahore, Pakistan
03:15-03:30 pm PST	Photocatalytic degradation of Metribuzin by Lab prepared mixed Oxide of Ti and Zn in aqueous solution	Dr. Atta ul Haq	Department of Chemistry, Government College University Faisalabad
03:30-03:45 pm PST	Plant-Mediated Biosynthesis of Zinc Oxide Nanoparticles For Remediation Of Acid Blue A Dye	Dr. Shumaila Kiran	Department of Applied Chemistry, Government College University, Faisalabad
03:45-04:00 pm PST	Antioxidant, Antidiabetic, Antimicrobial, Antihemolytic Activities of Gymnema sylvestre Leaves Extracts and Chemical Characterization – A Nanotechnology Approach	Memoona Ashraf	Department of Biochemistry, Faculty of Sciences, University of Agriculture, Faisalabad,
04:00-04:15 pm PST	Preparation of Silica Aerogel/Glass Fiber Composites and role of Supercritical CO_2 drying	Dr. Sameera Shafi	Institute of Chemistry, The Islamia University of Bahawalpur,Bahawalnagar Campus
04:15-04:30 pm PST	Creating water-repellent effects on pine wood by TiO_2 incorporated fluorocarbon impregnations	Kinza Hassan	Department of Physics, University of Agriculture Faisalabad
04:30-04:45 pm PST	Photovoltaic Properties of	Munawar Iqbal	Department of

	ZnO Films Co-Doped with Mn and La to Enhance Solar Cell Efficiency		Chemistry, The University of Lahore, Lahore 53700, Pakistan
Dinner/Fun Gala Library Ground, UE Faisalabad Campus. 08:00-10:00 pm PST			

Day-II
15th March January 2022

Timeline			
Registration Library Entrance, UE Faisalabad Campus. 8:00am PST			
Day-II Proceedings. Main Hall, UE Faisalabad Campus.			
09:00-09:15 am PST	Recitation from the Holy Quran Mr. Hafiz Muhammad Mazhar Iqbal Naat-e-Rasool e Maqbool by Ms Fareeha Ashraf		
Plenary Lectures Main Hall, UE Faisalabad Campus 09:15-10:45 am PST Chair: Prof. Dr. Muhammad Shahid Iqbal, Department of Chemistry, UE Jauharabad Campus Co-Chair: Dr. Imran, Department of Pharmacology, Faculty of Pharmacy, BZU, Multan Session Convener: Dr. Aeysha Sultan and Dr Ishrat Asghar, University of Education, Faisalabad.			
09:15-09:45 am PST	Prof. Dr. Afaq Ahmad, Center of Excellence in Solid State Physics, University of the Punjab, Lahore.		
09:45-10:15 am PST	Prof. Dr. Muhammad Saeed Iqbal. Inorganic & Analytical Chemistry, Drug Delivery Materials Forman Christian College. Lahore.		
10:15-10:45 am PST	Prof. Dr. Muhammad Babar Imran (TI), Director Punjab Institute of Nuclear Medicine (PINUM) Faisalabad.		
Tea Break Library Ground, UE Faisalabad Campus 10:45-11:15 am PST.			
Parallel Session-I: Online-I Room A29, UE Faisalabad Campus. 11:15-02:00 pm PST Session Convener: Dr Ishrat Asghar, Dr. Zahid Farooq, University of Education, Faisalabad			
Time	**Topic**	**Presenter**	**Affiliation**
11:15-11:30 am PST	Production of Gallic acid under solid-state	Dr Shagufta Saeed (**invited speaker**)	Institute of Biochemistry and

	fermentation by utilizing waste from food processing industries		Biotechnology, University of veterinary and animal sciences, Lahore
11:30-11:45 am PST	Assembly of CNTs Coated Stretchable Fabric for the Fabrication of Wearable Strain Sensors	Dr Zaka Ullah (**invited speaker**)	Department of Physics, Division of Science and Technology, University of Education, Lahore, 54770, Pakistan
11:45-12:00 pm PST	Optimized production of biodiesel from non-edible (tamarindus indica) seed oil.	Dr Noreen Sajjad, (**invited speaker**)	Department of Chemistry, University of Lahore
12:00-12:15 pm PST	Synthesis and Characterization of Lanthanum Substituted Manganese Spinel Ferrite ($MnLa_xFe_{2-x}O_4$) Nanoparticles	Kiran Naz	Institute of Space Science and Technology, University of Karachi, Karachi, Pakistan
12:15-12:30 pm PST	Structural, dielectric, impedance and electric modulus properties of Ni0.5Mn0.5Fe2O4/La0 2Bi0.8FeO4 nanocomposites	Arif Akhtar	Department of Physics, University of Karachi, Karachi, Pakistan
12:30-12:45 pm PST	Study of Neodymium ion (Nd^{+3}) doped Manganese-Cobalt (Mn-Co) mixed spinel ferrite nanoparticles for Energy Storage Applications	Junaid Kareem Khan	Department of Physics, NED University of Engineering and Technology, Karachi,
12:45-01:00 pm PST	Synthesis and characterization of (x)Cu0.05Co0.95Fe2O4/(1-x)La0.15Bi0.85FeO3 Nanocomposites	Muhammad Kashif	Department of Physics, University of Karachi, Karachi
12:45-01:15 pm PST	Synthesis and characterization of $(x)Cu_{0.05}Co_{0.95}Fe_2O_4/(1–x)La_{0.15}Bi_{0.85}FeO_3$	Ghulam Mustafa	Department of Physics, NED University of Engineering and

	Effect of Ce^{+3} doping on structural, magnetic, and electrical properties of Manganese-Zinc (Mn-Zn) mixed spinel ferrite nanoparticles		Technology, Karachi,
Parallel Session II: Organic & Biochemistry Main Hall, UE Faisalabad Campus. 11:15-02:00 pm PST Chair: Dr. Muhammad Shahid, Department of Biochemistry, UAF Co-Chair: Dr. Imran, Department of Pharmacology, Faculty of Pharmacy, BZU, Multan Session Convener: Dr. Muhammad Yaseen, Dr. Aeysha Sultan, University of Education, Faisalabad Campus.			
Time	**Topic**	**Presenter**	**Affiliation**
11:15-11:30 am PST	Extraction, modification and characterization of date palm mucilage to evaluate their therapeutic attributes	Dr. Muhammad Shahid, (**Keynote speaker**)	Department of Biochemistry, University of Agriculture, Faisalabad
11:30-11:45 am PST	Grewia asiatica juice supplementation exhibits anti-amnesic effects via modulation of cholinesterases and redox imbalance in the brains of scopolamine-amnesic Sprague Dawley rats	Dr Imran Imran (**Invited speaker**)	Department of Pharmacology, Faculty of Pharmacy, Bahauddin Zakariya University, Multan
11:45-12:00 pm PST	Synthesis and biological evaluation of novel ciprofloxacin derivatives as potential antitumor agents	Dr Ameer Fawad Zahoor	Department of Chemistry, Government College University Faisalabad
12:00-12:15 pm PST	A Greener Approach Towards Peptoid Modification Chemistry	Dr Akbar Ali	Department of Chemistry, Government College University, Faisalabad.
12:15-12:30 pm PST	Chitosan nanoparticles coated with curcumin as seed priming agents induce stress tolerance in wheat (Triticum aestivum L.) for sustainable growth	Dr Tahir Farooq	Department of Applied Chemistry, Government College University Faisalabad
12:30-12:45 pm PST	Mutagenicity, cytotoxic and antioxidant activities of	Dr Mazhar Abbas	Department of Basic Sciences

	Ricinus communis different parts		(Section Biochemistry), College of Veterinary and Animal Sciences, Jhang Campus-
12:45-01:00 pm PST	Exploration of recombinant papase as a new strategy to combat Dengue virus	Dr Abdul Ghaffar	Department of Biochemistry, Government College University Faisalabad
01:00-01:15 pm PST	Enzyme catalyzed synthesis of new and bioactive molecules	Dr Salman Zafar	Institute of Chemical Sciences, University of Peshawar, Peshawar
01:15-01:30 pm PST	Dyes adsorption by hydroxyethyl cellulose grafted with copolymer of polyaniline and polypyrrole	Dr. Muhammad Naveed	Department of Chemistry, Government College University Faisalabad
01:30-01:45 pm PST	Solubilization study of metal fluoride complexes of Nickel, Cobalt and Copper in anionic micellar media by conductometery and spectroscopic techniques.	Tehreem Naz	Department of Chemistry, University of Agriculture, Faislabad.

Parallel Session III: Inorganic, Analytical & Physical Chemistry

Room A28, UE Faisalabad Campus.
11:15-02:00 pm PST
Chair: Dr Muhammad Asif Hanif, Department of Chemistry, UAF
Co-Chair: Dr. Shahzad Zafar Iqbal, Department of Applied Chemistry, GCUF
Session Convener: Dr Naveed Ahmad, Dr. Hafiz M. Abdul Qayyum, University of Education, Faisalabad Campus.

Time	**Topic**	**Presenter**	**Affiliation**
11:15-11:45 am PST	Improved Spectrophotometric method for fast and accurate quantitative determination of menthol in essential oils.	Dr. Muhammad Asif Hanif **(invited Speaker)**	Department of Chemistry, University of Agriculture, Faisalabad.
11:45-12:00 pm PST	Storage effect in the levels of aflatoxins in	Dr. Shahzad Zafar Iqbal	Department of Applied Chemistry,

	selected edible seeds samples from, central cities of Punjab, Pakistan		Government College University, Faisalabad; Food Toxicology Lab, Plant Protection Division, NIAB, Faisalabad,
12:00-12:15 pm PST	Water splitting: design strategies (selected examples) challenges and way forward	Dr. M. Abdullah Khan	Renewable Energy Advancement Laboratory, Department of Environmental Sciences, Quaid-i-Azam, University, Islamabad
12:15-12:30 pm PST	Evaluation of Bis-(2-ethylhexyl) phthalate from Lactobacillus plantarum BCH-1 by using GC-MS and ESI-MS/MS	Dr. Mahwish Salman	Department of Biochemistry, Government College University Faisalabad, Pakistan
12:30-12:45 pm PST	Biochemical potential of Eucalyptus camaldulensis essential oils extracted by traditional and superheated steam extraction.	Dr. Muhammad Adnan Ayub	Department of Chemistry, University of Sahiwal, Sahiwal, Pakistan
12:45-01:00 pm PST	Chitosan nanoparticles coated with Moringa Oleifera extract as nano priming irfagent for physiological and biochemical alterations in wheat seeds	Dr. Arruje Hameed	Department of Biochemistry, Government College University Faisalabad
01:00-01:15 pm PST	Increased Cl - /SO_4^{2-} dialysis selectivity through polyelectrolyte multilayers coated aliphatic polyamide anion-exchange membranes	Dr. Muhammad Ahmad	Department of Chemistry, Division of Science and Technology, University of Education, Lahore
01:15-01:30 pm PST	Assessment of different extraction parameters on phytochemical constituent's profile and	Dr. Syed Ali Raza Naqvi	Govt College University Faisalabad, Pakistan

	antioxidant Potential of Dried Phlomis stwarrttii stem extract.		
01:30-01:45 pm PST	Phytochemical Analysis of Different Extracts of Moringa Oleifera Seeds and Leaves	Razia Noreen	Department of Biochemistry, Government College University, Faisalabad

Parallel Session IV: Theoretical & Applied Physics

Video Conference Room, UE Faisalabad Campus.
11:15-02:00 pm PST

Chair: Dr. Muhammad Yaseen Department of Physics, UAF
Co-Chair: Dr. Muhammad Irfan Majeed, Department of Chemistry, University of Agriculture Faisalabad
Session Convener: Ms Ambreen Aslam, Dr Ishrat Asghar, University of Education, Faisalabad Campus.

Time	Topic	Presenter	Affiliation
11:15-11:45 am PST	Influence of transition metal on the structural, electronic, magnetic and optical properties of SrTiO 3 perovskite	Dr. Muhammad Yaseen **(Invited Speaker)**	Department of Physics, University of Agriculture, Faisalabad.
11:45-12:00 pm PST	Molecular dynamics simulations of Dynamical Analysis in Weakly Coupled Dusty Plasmas	Rabia Waris	Modeling and Simulation Laboratory, Department of Physics, Government College University, Faisalabad
12:00-12:15 pm PST	Thermal conductivity of single-walled carbon nanotubes using molecular dynamics simulations	Ama tul Zahra	Modeling and Simulation Laboratory, Department of Physics, Government College University, Faisalabad
12:15-12:30 pm PST	Application of Surface-enhanced Raman Spectroscopy for Pharmaceutical sciences	Dr. Muhammad Irfan Majeed	Department of Chemistry, University of Agriculture Faisalabad

12:30-12:45 pm PST	Theoretical Investigations of TPA-DCPP Based Derivatives via Structural Modification of Donor Fragment	Dr Aftab Hussain	Centre of physical Chemistry, School of Chemistry, University of the Punjab, Lahore,
12:45-01:00 pm PST	Soft tissue and water substitute for megavoltage photon beams: An EGSnrc based evaluation	Ambreen Aslam	Department of Physics, University of Education, Lahore, Faisalabad Campus.
01:00-01:15 pm PST	The effect of laser irradiation on germination and seedling growth of Brinjal seed (Solanum melongena)	Sania Arif	Department of physics, University of Agriculture, Faisalabad-38000, pakistan.

Parallel Session V: Material Sciences

Room A32, UE Faisalabad Campus.
11:15-02:00 pm PST
Chair: Dr. Haq Nawaz, Department of Chemistry, UAF
Co-Chair: Dr. Ismat Bibi, Institute of Chemistry, The Islamia University of Bahawalpur, Bahawalpur
Session Convener: Dr. Munawar Iqbal, Dr G.M. Mustafa, Dr. Zahid Farooq, University of Education, Faisalabad Campus.

Time	**Topic**	**Presenter**	**Affiliation**
11:45-12:15 pm PST	Application of Surface-enhanced Raman Spectroscopy for disease diagnosis	Dr. Haq Nawaz (**Keynote speaker**)	Department of Chemistry, University of Agriculture Faisalabad
12:15-12:30 pm PST	Exploration and tuning of intrinsic mobility and optoelectronic properties of organic semiconductor materials	Dr. Ahmad Irfan **(Invited Speaker)**	Department of Chemistry, College of Science, King Khalid University, Abha, Saudi Arabia
12:30-12:45 pm PST	Highly Efficient ZnO Nanorods as an Adsorbent for Cr (VI) Removal from Aqueous Solution	Anila Tabassum	School of Chemistry, University of the Punjab, Lahore
12:45-01:00 pm PST	Effective photocatalytic degradation of Methylene	Ifra Shaheen	School of Chemistry,

	Blue dye in waste water system using Manganese Ferrite Magnetic Nanoparticles		University of the Punjab, Lahore, Pakistan
01:00-01:15 pm PST	Photocatalytic performance of doped and undoped Strontium hexaferrite nanomaterials and their structural, morphological and dielectric properties	Dr. Ismat Bibi	Institute of Chemistry, The Islamia University of Bahawalpur, Bahawalpur
01:15-01:30 pm PST	Synthesis , Characterization and therapeutic potential of ZnO nanoparticles from *Catharanthus roseus* leaf extracts	Dr. Naheed Akhter	Department of Chemistry, Government College University, Faisalabad.
01:30-01:45 pm PST	Efficacy of soil and foliar applications of chemically synthesized ZnO Nano fertilizer on morphological and nutritional quality of Zea mays crop: A comparison.	Muhammad Azam	Department of Chemistry, University of Agriculture, Faisalabad-Pakistan
01:45-2:00 pm PST	Improving the Structural, Optical and Photovoltaic Properties of Sb- and Bi-Co-Doped $MAPbBr_3$ Perovskite Solar Cell	Muhammad Iftikhar Khan	Department of Physics, The University of Lahore, Lahore 53700, Pakistan
Closing Ceremony Main Hall, UE Faisalabad Campus. 2:00-2:45 Convener: Dr. Muhammad Yaseen, University of Education, Faisalabad Campus.			
02:00-02:20 pm PST	Distribution of Certificates/Shields		
02:20-02:30 pm PST	Vote of Thanks by Prof. Dr. Muhammad Abid Rashid Principal University of Education, Faisalabad Campus		
02:30-02:40 pm PST	Remarks by Director S & T University of Education, Lahore		
02:40-02:45 pm PST	National Anthem		

Lunch and Prayer Break Library ground, UE Faisalabad Campus. 2:45-3:30 pm PST	
Parallel Session: Online-I Room A29, UE Faisalabad Campus. 03:30 pm-06:30 pm PST Session Convener: Dr Ishrat Asghar, Dr. Zahid Farooq, University of Education, Faisalabad Campus.	
03:30-04:00 pm PST	Dr. Eiasha Waheed, High Energy Accelerator Research Organization, Tsukubo, Japan.
04:00-04:30 pm PST	Prof. Dr. Dildar Ahmed, Department of Chemistry, FC College Lahore.
04:30-05:00 pm PST	Dr. Irfan Ahmad, King Khalid University, Abha, Saudi Arabia
05:00-05:30 pm PST	Prof. Dr. Shahid Atiq, Center of Excellence in Solid State Physics, University of the Punjab, Lahore.
05:30-06:00 pm PST	Prof. Dr. Jamshed Iqbal (TI), Head of Center of Advanced Drug Research, COMSATS Abbotabad.
06:00-06:30 pm PST	Prof. Dr. Farooq Anwar, Director Institute of Chemistry, University of Sargodha, Sargodha.

PLENARY LECTURES

PL02

Synthesis of novel drug candidates as urease inhibitors

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Abstract

Urease (urea amidohydrolase EC 3.5.1.5), the only Ni-containing metalloenzyme in eukaryotes, is widespread in nature, and found in a variety of plants, algae, fungi, and bacteria. It catalyzes the hydrolysis of urea to ammonia (NH_3) and carbon dioxide (CO_2). Liberation of ammonia increases pH significantly and allows the bacteria to survive during colonization. During Helicobacter pylori (H. pylori) infection, the increase of stomach pH is considered as a root cause of pathologies of gastric ulcers. Therefore, it is a common notion that ureases are involved directly in the pathogenesis of several diseases such as peptic and gastric ulcer, pyelonephritis, urolithiasis, ammonia and hepatic encephalopathy, hepatic coma and urinary catheter encrustation. The gastric and peptic ulcers, sometimes may lead to cancer. Hyperactivity of urease brings out considerable economic and environmental tribulations by releasing abnormally large quantity of ammonia into the atmosphere in the process of urea fertilization. To date, only acetohydroxamic acid, has been clinically used for the treatment of urinary tract infections by urease inhibition. In the current situation, the increasing resistance of bacterial pathogens to common antibiotics is the alarming situation for researchers working in this field. Therefore, it is foremost task to develop the novel classes of molecules that specifically target urease as enzyme inhibitors. Our research group has successfully identified a range of lead molecules for the inhibition of urease enzyme. Interesting results our research on urease inhibitors would be presented.

PL03

Endocrine Disrupting Chemicals in Fresh and Marine Aquatic Environments

Yuegang Zuo

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Abstract

Endocrine disrupting chemicals, particularly the synthetic and natural estrogenic steroids such as ethinylestradiol (EE2), mestranol(MeEE2), estrone(E1), estradiol(E2) and estriol(E3), and plasticizers such as bisphenol A (BPA) and phthalate esters, have attracted a great deal of scientific and public attention during recent years due to their occurrence in surface waters and sewage treatment plant effluents and their potential adverse effects on the development and reproduction of fish, wildlife and even human beings. In this presentation, we will focus on our research on the occurrence, sources, bioeffects, and microbial and photochemical degradation of both synthetic and natural estrogenic steroids and plasticizers in fresh and marine aquatic environments during the past decade. To face analytical challenges for determining trace amounts of estrogenic steroids and plasticizers in natural waters, GC-MS and HPLC analytical methods have been developed. The developed methods were applied to the water samples periodically collected from wastewater treatment plants, lakes, Acushnet River and Buzzards Bay. The interested compounds were detected in water samples in nano- to micro-gram per liter concentration range, in which can certainly cause fish feminization and may also contribute to the observed declines in lobster population in Buzzards Bay. Microbial and photochemical degradation of E1, E2, E3, EE2 and MeEE2 have been also investigated in seawater as well as in waste, lake and river waters as a comparison. The microbial degradation of synthetic steroid estrogens is extremely slow with a half-life of longer than 70 days in seawater. However, the photodegradation of these compounds are much faster with a half-life of 17 hours for EE2 and 19 hours for MeEE2. Humic and other dissolved organic substances significantly accelerate the sunlight-induced photodegradation of estrogenic steroids. Transition metal Fe(III), nitrate and nitrite can further catalyze the photochemical decomposition of these steroids.

PL04	

The next wave of photonics innovations in the sciences, arts and engineering

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Abstract

Photonics, (the science and engineering of the photon) has been identified as one of the most prominent cutting-edge fields in science and technology for the 21st century. Photonics involves cutting-edge uses of lasers, optics, fiber-optics, and electro-optical devices in numerous and diverse fields of technology. It is playing an increasingly important role in science and engineering today. Since the invention of the laser, there has been extensive growth, and prolific research and development in this area. Entirely new fields within applied science and technology, such as, laser materials processing, optical remote sensing, nonlinear optics, fiber optics, photonic networks, biophotonics, organic photonics, integrated photonics, silicon photonics, etc., have opened up, and old subfields of engineering have been greatly extended with the introduction of photonics. Individuals with advanced training and education in photonics engineering are in greater demand today than ever before. There are more jobs and challenging technical positions in both government and industrial sectors for work in photonics. Applications to military and non-military problems are much more numerous. The 21st century will depend as much on photonics as the 20th century depended on electronics [1].Therefore, need for individuals who are qualified to work in photonics engineering is at an all-time high, and that demand will increase with technological advancement. According to a report by United Nations Industrial Development Organization (UNIDO) and the International Centre for Science and High Technology (ICS), the photonics engineers have great scope in establishing small and medium enterprises (SMEs) [2].They will also be able to continue their education toward an MS or a PhD degree in numerous areas of modern optics, laser manufacturing, optoelectronics, photonics networks, software development, instrumentation & control, nanotechnology, bio photonics, etc. In this talk, the next wave of photonics innovations in the sciences, arts and engineering will be unveiled, major challenges, the future prospects of these innovations and their importance for Pakistan will discussed.

References

[1] N. R. Council, Optics and photonics: Essential technologies for our nation: National Academies Press, 2013.
[2] N. Drago and P. Villoresi, "Graziano Bertogli, Laser technologies: a step forward for small and medium Enterprises, International Centre for Science and High Technology, Trieste," ed, 2008.

PL05

What is Mass?

Dr. Faisal Akram
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Abstract

Ever since the dawn of civilization on Earth, humans have always thought of mass as an intrinsic property of a material substance. The relatively recent understanding that all material substances are made of some fundamental particles just shifts the problem of understanding the nature of mass from substance to its constitutions. However, recent developments in understanding the nature of particles and their interactions, that have culminated into the standard model of particle physics have revolutionized our understanding of mass. Mass is not an intrinsic property of a material substance. It is not something that matter just has. It is a behavior of the quantum fields. It is something that they do. The objective of this talk is to explain to a general audience this new understanding of the nature of mass.

PL06

Gold – from Jewelry to Medicine

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Abstract

Gold is one of the noble metals known to man at an early stage. It finds attractive applications as metal; however, little is known to common man about its potential in medicine. Some of the gold salts have been used to treat tuberculosis in ancient times. In the 20th century fascinating chemistry evolved in favor of gold compounds for treatment of rheumatoid arthritis. Now gold chemistry has entered new era of cancer therapy, treatment of amebiasis and nanomedicine. This lecture will highlight some of the salient features of journey of gold from jewelry to medicine.

PL07

How Sciences manifest in medicine

Muhammad Babar Imran
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Abstract

The existence of the universe is explained by two entities: matter and energy. These two entities are interchangeable and exist in different forms to make up all things visible or invisible in the universe. Energy can exist in several forms and one form can change to another form. Radiation is one of the forms of energy and has great importance in nuclear medicine. It is emitted by one object and absorbed or scattered by another. Attempting to understand the nuclear medicine, needs clear understanding of the scientific basis of nuclear medicine through basic laws of physics, chemistry and biology. All these sciences are interlinked and we only align them to meet the challenges faced while conducting nuclear medicine research, and also to foreseeable new technologies and opportunities for personalized health care. Starting from atom and its basic structure to the development of nuclear reactors and particle accelerators that produce radionuclides, chemical processes to synthesize radiopharmaceuticals used for imaging and treatment; and instruments that can detect radiation emitted from the radionuclides that accumulate in the human body, basic sciences are involved and playing its role in understanding and managing the disease. The two major components of nuclear medicine imaging procedures are radiopharmaceuticals and the imaging system. The radiopharmaceuticals are designed for tracing pathophysiologic and molecular disorders. Radioisotopes undergo radioactive decay and utilize the penetrating capability of gamma rays to functionally map the distribution of the administered compound within different biological tissues. The imaging systems, i.e, scintillation cameras or positron emission tomographic (PET) scanners have passed through a number of developments since their introduction in the late 1960s and have had a significant impact on the diagnostic quality of nuclear medicine. The understanding of their working principles starts from coulomb interactions, light particles versus heavy particles and their stopping power and range

PL08

Transfer matrix method and optical properties of a thin-film

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Abstract

The transfer matrix method is widely used to investigate the wave propagation through a thin-film and multilayer structures. This method along with the Lorentz oscillator model is used to find the transmittance of a thin-film SrTiO 3 and then other optical properties like refractive index, absorption coefficient and optical band gap are deduced from it. These theoretical calculations are compared with the experimental findings.

KEYNOTE LECTURES

KN01

Ablative Laser Propulsion in single and multilayered targets.

Dr. Yasir Jamil
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Abstract

Impulse imparted by pulsed laser ablation of a thin layer of material creating a plasma or vapor is an interesting concept that allows for scaling of the induced thrust over a large range by selecting an ablation laser of appropriate pulse energy and repetition rate. Its potential for the removal of space debris using a high energy laser and for laser ablative microthrusters which produce highly precise thrust in the μN range at μJ to mJ pulse energies. This talk will provide an overview of the research regarding ablative laser propulsion in single and multilayered targets, which have been set up at UAF, Faisalabad to further investigate the potential of both of these applications of laser ablative propulsion. It has been demonstrated that laser ablative thrusters can produce μN thrust levels at high specific impulse and have the capability of producing very low minimum impulse bits down to nNs range in single shot operation. So far these concepts have been based on providing unablated material at each laser pulse by implementing a propellant feed mechanism or using a liquid propellant.

KN02

Applications of Computational Methods in Drug Design

Zaheer Ul-Haq
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Abstract

Drug discovery is one of the most important processes in the pharmaceutical industry. With the rapid development of both computer hardware, software, and algorithms, drug designing have benefited much from various computational methods which greatly reduce the time and cost of drug development. In this talk, I will use few examples from our ongoing research projects to discussed the roles of biomolecular simulations in identifying drug binding sites on the target macromolecule and elucidating drug action mechanisms. Then, virtual screening methods (e.g., molecular docking, pharmacophore modeling, and QSAR) as well as structure- and ligand-based drug design were discussed in detail.

KN03

The electroweak unification, and the weak neutral current

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Abstract

After introducing weak interactions and its first Fermi model without an exchanged particle, the talk is to acquaint with the standard model having an exchanged particle. For low energies, this general model becomes the Fermi model and for large energies the same model becomes the usual quantum electrodynamics whose exchanged particle (photon) has with zero rest mass. An innovation recognized through a few Nobel prizes showed how the exchanged particle of the standard electroweak model can have a non-zero rest mass, while still obeying the essential requirement of gauge invariance that generalizes the condition that adding a constant to potential energy does not change physical predictions. In addition to predicting the recently discovered Higgs particle, this

electroweak unified theory had a novel prediction earlier verified in the form of an exchange of the massive Z particle.

KN04

Multi-omics approach for Biomarker search using Advanced Mass Spectrometric Tools: understanding the progression of Preleukemic diseases towards Leukemia-as a case study

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Abstract

Multi-omics approach particularly use of proteomics and metabolomics by advanced mass spectrometric tools has a potential to be used for biomarker discovery in epidemiology and personalized medicine. Two sub-classes of acute leukemia including acute lymphoblastic leukemia (ALL) and acute myeloid leukemia (AML) with two preleukemic diseases, aplastic anemia (APA) and myelodysplastic syndrome (MDS) and healthy individuals were analyzed by modern spectrometric techniques and compared. ALL is the most common form of leukemia in children that also occurs in adults around the age of 50 with low incidence rate. AML, is leukemia of all ages which is of two types; primary which occurs de-novo and secondary which can occur after MDS, other myeloproliferative disorders and after chemotherapy. Aplastic anemia (APA) and myelodysplastic syndrome (MDS); two preleukemic diseases have been reported to proceed the AML insome case studies. Metabolic studies were performed using gas chromatography triple quadruple mass spectrometry. GC coupled with triple quadrupole tandem MS and multivariate statistical analyses for sample and data analyses, respectively. Methods were previously developed and optimized by our research group[1]. Twenty seven out of 1425 metabolites were found differentiative among ALL, AML, aplastic anemia (APA) patients and healthy control using p-value $\leq$ 0.001. ALL is the most dissimilar group from other three groups as in hierarchical clustering showed 72.1% dissimilarity. Model generation using PLSDA gave an overall accuracy of 91.9%. Based on pathways analysis, fatty acid metabolism is deregulated in patients with AL and may represent an underlying metabolic pathway associated with disease progression[2]. Metabolites were also investigated in these samples by using ^{1}H NMR (nuclear magnetic resonance) spectroscopy in which thirty-seven putative metabolites were identified using Carr-Purcell-Meiboom-Gill (CPMG) sequence[3]. In the proteomics strategy, a multi-fractionation approach was used for the fractionation of pooled plasma samples of all study groups[4]. Up-and down-fold changes in concentration of proteins were observed in two-dimensional gel electrophoresis (2D-GE) gels of diseases in comparison to healthy.Among 34 identified proteins, eightproteins which were significantly deregulated include serum amyloid A-1 (SAA1), haptoglobin (HPT), C4b-binding protein alpha chain, complement factor 7, apolipoprotein E (ApoE), plasminogen, prothrombin, and complement factor H (CFH), and their links were found to important cell signaling pathways.Validation through ELISA showed that SAA1 and plasminogen may be considered as potential molecules to link leukemia with APA and MDS.Combinedly these studies helped in early diagnosis and linking progression of leukemia at high significance levels by only serum analysis. The developed method successfully provided the molecular insight into this progression and identification of the metabolomics and proteomic molecules that can associate preleukemic diseases to leukemia. Details will be discussed in the lecture.

References

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2. Musharraf, S.G. et al. (2016) SERUM metabolomics of acute lymphoblastic leukaemia and acute myeloid leukaemia for probing biomarker molecules. Hematological oncology.
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KN05

Extraction, modification and characterization of date palm mucilage to evaluate their therapeutic attributes

Muhammad Shahid[1], Fozia Anjum[2*], Samreen Gul Khan[2], Naheed Akhter[3]
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Abstract

A green synthesis route was reported to explore the modification, reducing and capping potential of Phoenix dactylifera mucilage for the synthesis of silver nanoparticles. Nucleation process and synthesis of silver nanoparticles were monitored by taking the UV/ VIS absorption spectra during the reaction. Antioxidant, medicinal potential as well as cytotoxicity of crude and modified mucilage were also analyzed. Synthesized spherical nanoparticles were sized up to 39nm. UV/VIS spectroscopic results revealed an intense peak at 427nm along with other small peaks in region 350-450 nm owing to the existence of poly disperse silver nanoparticles. Maximum phenolic contents were displayed by crude mucilage (230.37 ± 0.04 mg). Scavenging activity (44.18 ± 0.95) and flavonoid contents (28.47 ± 0.07) was detected maximum in carboxymethylated mucilage. Nano formulated mucilage exhibited bactericidal activity maximum against Escherichia coli and minimum against Staphylococcus aureus and inhibition zone was calculated up to 35 and 17mm respectively. Growth inhibition (F. solani & A. niger) by nano formulated date palm mucilage was maximum (45.00 & 66.67%) of all the samples under investigations. The outcome exposed that such modified products may have potential applications in food as well as medicaments.

KN06

Application of Surface-enhanced Raman Spectroscopy for disease diagnosis

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Abstract

Different diseases are the major reason for the number of deaths globally. Primary diagnosis and treatments now have become productive routes for the control of increased death rates. There are huge challenges for detecting severe diseases with better sensitivity. In the modern years, surface-enhanced Raman spectroscopy (SERS) appeared as the most popular practice for the detection of different diseases like Cancer, Hepatitis, Tuberculosis, Diabetes, etc. SERS identifies diseases with great efficiency and potential for clinical detection. To collect different spectra, the required samples are examined by applying the SERS technique. After the collection of no. of spectra, different statistical tools are used like PLDA, PLSR, etc using computational software. In this field, very effective work has been done in the current 5 years
and there are future challenges as well.

Keywords: Raman Spectroscopy; SERS; Disease Detection; spectroscopic analysis; Cancer; Hepatitis; Diabetes; tuberculosis; biomolecules; multivariate data analysis

KN07

Influence of transition metal on the structural, electronic, magnetic and optical properties of SrTiO 3 perovskite compound: First principles calculations

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Abstract

First principles investigations are performed on electronic, optical and magnetic properties of Sr1-xVxTiO3 at x 0% 12.5%, 25%,50% and 75% by using density functional theory calculations. The formation energy is used to confirm the stability of ferromagnetic phase. The calculated results shows that the spin-dependent electronic band structure and density of states exhibit half metallic behavior for all concentration and semiconductor nature for pristine compound. Thenmagnetic study shows that the main contribution to the magnetic moment is mainly from the vanadium atom. Furthermore, the optical parameters including dielectric function, absorption coefficient, reflectivity and refractive index are calculated within 0-10 eV energy range. The outcomes reflect potential applications of Sr1-xVxTiO3 in optoelectronic and spintronic applications.

Parallel Session I: Online Session

OL-01

Applications of Laser Induced Breakdown Spectroscopy

Prof Dr Arif Demir

Laser-induced breakdown spectroscopy is a useful research and analysis tool. LIBS analysis is a versatile approach because it can be used on any kind of material, whether solid, liquid, or gas, and will detect any and all chemical elements in a sample with a single pulse. LIBS is especially sensitive in the detection of light elements that are not easily detected by other analytic methods. Valuable progress has been made during the last few years on very diverse and versatile applications of LIBS, including remote material assessment, geological analysis in space exploration, diagnostics of archaeological objects, metal diffusion in solar cells. In addition to vast applications in medical and biological sciences. Laser-induced breakdown spectroscopy (LIBS) has been utilized for in situ diagnostics of the laser welding process.

OL-02

Assessment of broad inhibitory potency of endemic *Turanecio hypochionaeus*: Phenolic contents and bioactivities with in silico studies

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Abstract

Plants are natural resources used to cure various diseases or alleviate their symptoms from ancient times. The use of folkloric plants in traditional treatment methods is more preferred in underdeveloped or developing countries. Considering Turkey's floristic richness, traditional medicine is of great importance and contains many medicinal plants. Turanecio genus, members of the Asteraceae family, is an endemic plant that grows naturally in Turkey. *Turanecio hypochionaeus* species, which is endemic to the flora of Turkey, has not yet had a traditional use reported. Since studies on the plant are extremely limited, this study aimed to quantify the phenolic content, screen the anti-cholinesterase, anti-diabetic, anti-urease, anti-melanogenesis, anti-lipase, and antibacterial properties activity of *T. hypochionaeus* collected from Bartın province (Turkey). The calculated IC_{50} values for the studied enzymes were between 0.234-116.50 µg mL^{-1}, and the plant extract inhibited HMG_CoA R and glycosidase enzymes more with IC_{50} values of 0.234 and 116.50 µg mL^{-1}, respectively. Among the 11 secondary metabolites identified in *T. hypochionaeus*, chlorogenic acid (255.459±1.17 µg g^{-1}), benzoic acid (56.251±1.98 µg g^{-1}) and catechin (29.029±0.27 µg g^{-1}) were determined as the most abundant phenolic compounds. Also, the plant extracts showed antimicrobial and antifungal properties in a dose-dependent manner according to the results of the tested

microorganisms. The interactions of the secondary metabolites extracted from the *T. hypochionaeus* plant against different enzymes were investigated with a molecular docking study. Chlorogenic acid was determined as the most active compound against HMG_CoA R and α-amylase, α-glycosidase, and lipase, and it has binding energies of -12.80, -12.80, -12.60, and -12.00 kcal/mol, respectively.

Keywords: Enzyme inhibition; molecular docking; phenolic compound; *Turanecio hypochionaeus*

Acknowledgments

This study was supported by the TÜBİTAK (The Scientific and Technological Research Council of Turkey) (Grand ID: 120Z005).

OL-03

Development of novel high-capacity sodium chromate/carbon nanocomposite anode for Sodium-ion batteries

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Abstract

With the increase of electricity production from renewable energy resources, large scale energy storage systems (ESS) are required to store the energy due to their intermittent nature. Sodium-ion batteries (SIBs) have recently re-emerged with the advantage of low cost and abundant resources of sodium. However, their commercialization requires high performance cathode and anode materials. Commonly used anode material in lithium-ion batteries such as graphite do not show sufficient performance in SIBs and hence, cannot be used. Therefore, high capacity anode materials with excellent stability are required for commercial SIBs. Here, a nanocomposite comprising of sodium chromate (Na 2 CrO 4) and acetylene black is synthesized using ball milling method. The prepared Na 2 CrO 4 /C nanocomposite shows a capacity of 228 mAh g -1 at a rate of 0.1 C. The Na 2 CrO 4 /C nanocomposite shows good capacity retention and delivered a capacity of
166 mAh g -1 at 100th cycle. The reaction mechanism of nanocomposite is explored using in-situ XRD which suggest transformation of crystalline to amorphous phase upon cycling. X-ray absorption spectroscopy was conducted to observe the redox change of Cr in the Na 2 CrO 4 /C nanocomposite.

OL-04

Construction of New Heterocycles via Indoles and Carbazoles

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Abstract

Nitrogen-containing heterocycles have been the subject of intense study and considerable effort has been devoted to the synthesis of these heterocyclic systems as they are found in a wide range of biologically active molecules and alkaloids. 1 Among these nitrogen containing heterocycles, indoles continue to play a central role in the development of new structures for both chemical and biological properties. They are the source of numerous biologically active natural products by virtue of their derivation from tryptophan units which are essential to peptide, protein and enzyme structures. Although the indole unit is electron rich and displays a wide range of reactivity, many naturally-occurring indoles contain methoxy substituents, which enhance their reactivity. The synthesis of methoxyindoles has also become a strategy for diversifying the regiochemical behaviour of indoles. More complex indoles, such as bis-indoles are also very important biologically active scaffolds as they are found in many pharmacologically active alkaloids. Bis-indole alkaloids are heterocyclic compounds, which consist of two indoles connected to each other via linking units. Carbazole is another important class of nitrogen containing aromatic heterocyclic compound and generally recognized as a significant structure in organic and medicinal chemistry. Apart from biological importance of carbazole derivatives; they are also used as useful building blocks for the synthesis of new organic materials and

play an important role in the area of electroactive and photoactive materials. More specifically, hetero-annulated carbazole alkaloids, such as pyrrolo-carbazoles scaffolds have attracted considerable research attention due to their distribution in numerous natural products with useful bioactivities.

OL-05

Cannabis (Marijuana) and Cannabinoids: Development of an Efficient Formulation for Cannabinoids Delivery

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Abstract

Cannabinoids are a group of substances found in the cannabis plant (Cannabis Sativa). Oral delivery of cannabinoids e.g. CBD and THC, for medicinal or recreational purposes, needs to develop efficient formulations. For this purpose, we developed SofTabs - an innovative formulation for cannabinoid and nutraceuticals delivery. It is a gelatin-based oil-water emulsions that dissolve in the mouth for sublingual adsorption of cannabinoids or can be chewed for oral adsorption. This technology was pioneered by a Norwegian company and SofTab Technologies Inc., based in Windsor (Canada, ON), that recently acquired the worldwide licence to use the technology for the production and distribution of cannabinoids SofTabs products. SofTabs formulations are homogenous emulsions in a viscoelastic state made from suspending the active ingredients or extracts in an appropriate gelatin/oil matrix allowing them to retain their shape and other physio-mechanical properties. This presentation will highlight the general strategy to prepare SofTabs and optimization of each step to get the desired products. SofTabs characterizations e.g. viscoelastic properties, water droplet size in emulsion and methods to test homogeneous distribution of the ingredients would also be discussed. SofTabs are easy to flavour and are readily tunable by simply modifying the balance of the ingredients. SofTabs cannabinoids products with different favours e.g. lemon, orange, strawberry etc. were prepared and their effect on the final mechanical properties was investigated. A related investigation, focusing on the incorporation of other supplements e.g. pain-relief pharmaceutical ingredients and vitamins will also be examined. As part of the project, vegetarian version of SofTabs using different types of carrageenan obtained from the red see-weed to replace gelatin was also investigated. Finally, shelf-stability of the products and processing conditions to ensure that the material would survive the manufacturing process intact and will support the establishment of the manufacturing plant will also be focused. SofTabs technology has a promising future in cannabinoids and nutraceutical delivery and in the drug formulations. Future plans e.g. investigation about bioavailability of the active ingredients and the scale-up of the processes and ensuring that analytical quality remains excellent, would also be discussed in this presentation.

OL-06 Dr Simon Rondeau-Gagne

Controlling the Thermomechanical Properties of Semiconducting Polymers Toward Stretchable Organic Electronics

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Email: srondeau@uwindsor.ca

Abstract

Materials processing and optimization is crucial for the development of next generation technologies, in which smart and conformable devices and sensors embedded ubiquitously will collect and exchange data continuously. In this context, known as the Internet of Things (IoT), materials not only require a good charge transport and processability in eco-friendly solvents, but also to be mechanically robust and stable to many different conditions. In recent years, important efforts have been devoted to push the boundaries between chemical engineering and chemistry towards materials with excellent charge transport. However, devices built from these materials still demonstrate some limitations which limit their use for the IoT. Therefore, it is critical to develop novel materials with improved

electronic and mechanical properties, and develop new strategies to obtain semiconducting materials that can tolerate various environmental conditions. To address this challenge, our group recently developed new stretchable semiconducting composites through physical blending of conjugated polymers with thermoplastics and elastomeric materials. This strategy exploits the many interesting properties of conjugated polymers, which are implemented to soft amorphous materials, such as polyethylene and polysiloxane. Due to the important difference in surface energy between the soft materials and the conjugated polymer, the two matrices are not miscible. Therefore, upon physical mixing, a phase separation occurs, creating segregated and isolated domains of conjugated polymers. This phase segregation in the solid-state is crucial; by confining the conjugated polymers into the stretchable matrix, a continuous conductive pathway forms, allowing for charges to move in the bulk without interruption. Moreover, the matrix is not altered, which allows for a preservation of the thermomechanical properties of the materials. This presentation will cover the preparation of new functional semiconducting polymers through the utilization of polymer blending as a strategy to design intrinsically stretchable semiconducting materials. Results from a detailed characterization of the solid-state morphology of the new materials in thin films will be introduced, as well as the new structure-property relationships unveiled during our investigations. Application of the materials as active materials in thin film transistors (TFTs) and flexible sensors will also be discussed

OL-07

Organometallic and Coordination Compounds and Their Potential Uses on Green Chemistry, Catalysis and as Metallodrugs

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Abstract

In this talk, we will address some recent advances from our laboratory regarding the synthesis, characterization, and uses of different kinds of coordination and organometallic compounds, being relevant the Pincer and NHC motifs. The exploration on the potential uses of isolated natural products as ligands will also be highlighted. Then, relevant results regarding the examination of the catalytic (e.g., cross coupling reactions) and cytotoxic (i.e., Cancer) activities of these complexes will be presented along with several points concerning the potential usage of more environmentally empathic solvents and potentially usable alternative energy sources.

OL-08

Physics prospects at the Belle II experiment

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Abstract

The Physics of the B Factories describes the quest for the precise determination of asymmetry, broken symmetry between particles and anti-particles. The results of B factory experiments such as Belle and BaBar, have confirmed the Standard Model (SM) picture of the quark flavor sector and the complex phase of the CKM matrix as the main source of the CP violation. The Belle II experiment which is successor of Belle experiment at the SuperKEKB e+e−collider started its operation in 2018, with the goal of collecting 50 ab−1 of data. This will allow for high precision measurements in the quark flavor sector, opening a window into physics at the energies beyond achievable at the high energy frontier experiments. I will present the recent status of the SuperKEKB and the Belle II experiment along with some physics prospects.

OL-09

Green chemistry: trends and prospects

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Abstract

With an ever-increasing realization of the potential safety and environmental concerns associated with the chemical processes and products, green chemistry has emerged as a novel platform for innovative research and development activities in chemistry. It is increasingly influencing almost all domains of chemistry, chemical engineering, and related fields of knowledge. Its impact can be witnessed in many areas of research in chemistry. There is an increasing emphasis on replacing harmful volatile organic solvents with safer alternatives. Efforts are underway to explore strategies to use water as a solvent for extraction of bioactive compounds from plants and other organisms, as well as for organic reactions. Synthesis and use of novel green solvents consisting of ionic liquids (ILs) and deep eutectic solvents (DESs) for extraction and synthesis is another area of active research. Solvent free extractions and reactions constitute an innovative field of research. Another area of active research is to explore greener techniques which can replace environmentally hazardous conventional ones. These include the techniques using microwave and ultrasound energy for extraction and synthesis, and no-solvent mechanochemical processes for organic synthesis. Innovations in green chemistry are important for sustainable environment. Efficiency, cost effectiveness and safety are other desirable aspects. The talk will focus on some of the emerging research areas of green chemistry with the objective to draw attention of the young chemists to this rapidly growing and promising field of research.

OL-10

Exploration and tuning of intrinsic mobility and optoelectronic properties of organic semiconductor materials

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Abstract

The organic π-conjugated materials have considerable interest in semiconductor devices. The organic semiconductor materials (OSMs) are efficient to be used in photovoltaics, organic field effect transistors, laser technology, electroluminescent and electronic devices. Numerous OSMs like polycyclic organic compounds are most important players in the field of electronics. We have explored the optoelectronic properties and intrinsic mobility of various compounds by advanced computational approaches then compared the data with experimental and/or computed evidence. Additionally, we have designed various new compounds by multiple strategies with the aim to tune their properties of interests. Effect of various functionals and basis sets was systematically studied and compared. The effect of donor (D), acceptor (A), π-bridge was investigated on the charge transport and optoelectronic properties at molecular and bulk scales e.g., frontier molecular orbitals (FMO), absorption, fluorescence, transfer integrals, electron affinity (EA), ionization energy (IE), reorganization energy, density of states, conductivity, dielectric functions, refractive indices and extinction coefficient. The hole and/or electron transfer nature of the OSMs was evaluated by shedding light on the transfer integrals, reorganization energies and intrinsic mobility. Some multifunctional materials were proposed with enhanced properties than parent compounds with anticipation that such compounds would be suitable to be used in semiconductor devices.

OL-11

A neoteric tri-phase composite with efficient magneto-electric and multifunctional response

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Abstract

Multiferroic materials have gained research limelight owing to their potential candidature for energy storage applications which are efficiently triggered by their intrinsic magnetoelectric effects. In this context, we present an efficient tri-phase multiferroic composite material, consisting of $BiFeO_3$, $CoFe_2O_4$ and Cr_2O_3 exhibiting exceptional viability for energy storage. The individual constituents were prepared by a citrate- gel based self-ignition route while the composite formation was routed through a ball-milling process. Diffraction patterns revealed the co-existence of three crystalline phases without any impurity within the composites. The morphological features directly influenced the dielectric parameters well in accordance with the Maxwell-Wagner's bilayer model and the Koop's phenomenological theory. Likewise, the Nyquist plot architecture a single semicircular arc specifying single relaxation phenomena. The insight of current versus voltage (I-V) curves through the multiferroic tester exposed a gradually declining trend of leakage current against the increasing Cr_2O_3 phase fractions. The PUND sequences represent high values of switching charge polarization (P*) as paralleled to the un-switching polarization which accompanies leakage current. Magnetic-hysteresis loops exposed a weak ferromagnetic nature of the samples and an increased Cr_2O_3 phase fractions did not significantly affect the coercivity (Hc) values. The ME-coupling effect was also evident from variation in polarization signals by applied magnetic field. The present study unveils an efficient, scalable and affordable pathway towards the substantial synthesis of tertiary-phase composites exhibiting superb storage properties.

OL-12

The therapeutic potential of purinergic receptors antagonists

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Abstract

P2X receptors are potential therapeutic targets for the treatment of various neurodegenerative disorders, pain, inflammation, hypertension, and cancer. Adamantane ring has been reported to exhibit significant inhibitory potential towards P2X receptors, especially for P2X7R. We have utilized uniqueness of adamantane moiety in our synthesized compounds and introduced various substitutions that enhanced the potency as well as selectivity for P2XR subtypes. Among synthesized derivatives, 4n and 5b were found to be most potent and selective inhibitors for h-P2X4R and h-P2X7R, respectively. 4n was found to be highly selective for h-P2X4R with IC 50 ± SEM= 0.04 ± 0.01 µM, that is 22 times more potent than BX-430, a standard selective inhibitor of h-P2X4R. 5b has IC 50 ± SEM of 0.073 ± 0.04 µM, which is comparable with the known antagonists of h-P2X7R. 4n and 5b were studied for mode of inhibition of P2XRs and both were found to be negative allosteric modulators. In silico studies were also conducted to find the type of interactions as well as mode of inhibition.

OL-13

Extraction of plant-based functional components using some green routes

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Abstract

A number of conventional techniques such as decoction, maceration, infusion, percolation, hydro-distillation and Soxhelt methods, involving the use of high volume of organic solvents and/or accelerated temperature, are often employed for the extraction of different plant bioactives/functional components (FC). However, there are serious concerns regarding the process safety and non-environment friendly nature of such techniques. Moreover, the quality of the end-use extracts thus produced is also questioable as far as food and therapeutic applications are concerned. Infact extraction of wide array of plant-based FC having different structural features and biological attributes is not possible using a single solvent or technique. In the modern era of optimal nutrition, now the functional food and

nutra-pharmaceutical industry is in demand of pure, non-denatured and healthy extracts. Hence, there is growing interest of researchers and food chemists in the developlment of alternatives green extraction which can yield better and pure food and nutra-pharma grade extracts. This lecture is mainly designed to highlight the principles and applications of emerging green extraction which can be used for the effective recovery of high-value FC from plant based materials. Some of our own research findings and methodological developments related to green extraction protocols such as enzyme-assisted extraction, ultrasound-assisted-extraction coupled with supercritical fluid extraction (SFE) are also presented. Especially, the improvement in extraction yield and nutraceutical quality of of lipids/vegetable oils and phenolic extracts is focused.

Parallel Session II: Organic & Biochemistry

O-COB-01

Labeling of linzolid with Tehnetium-99m and its biodistribution in Swiss Albino mice

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Abstract

Techenetium-99m is the most widely used radionuclide for diagnostic applications. Linezolid is an antibiotic of the oxazolidine group that is used to treat infections caused by multi resistant bacteria. The aim of this study was to label a linezolid with technetium-99m (Tc-99m) for diagnostic purpose. 99m Tc-linezolid injection was prepared using 1.5 mL of 99m Tc- pertechnetate with linezolid at pH 5 in presence of stannous chloride as reducing agent. The labeling efficiency of 99m Tc-linezolid injection was found to be greater than 98%. The 99m Tc-linezolid complex was stable up to 24 h at room temperature determined by paper chromatography and ITLC-SG. The charge on the 99m Tc-linezolid was determined by electrophoresis technique. The biodistribution study of 99m Tc-linezolid was carried out using male Swiss Albino mice

Keywords: 99m Tc-pertechnetate, Linezolid, electrophoresis and biodistribution

O-COB-02

Biotransformation of organic wastes into value-added products: recent developments and challenges

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Abstract

The prompt growth of the human population has enhanced the need for food, foodstuff, and chemicals that have escalated the dependency on the generation of organic wastes and fossil-based resources. Moreover, with the increasing economical, energy and environmental issues at global level, scientists have been considering attention in valorization of naturally occurring lignocellulosic-based materials. Valorization of organic waste has gained striking attention because of ease of accessibility, high abundance and renewability, thus serving as a potent approach for the waste management. Agro-industrial and food processing wastes are highly nutritious and contain many bioactive compounds. Agro-industrial wastes, such as rice bran, sugar cane bagasse and corn cob, have been widely investigated through different fermentation technologies for the enzyme production and many other useful commodities. With the advancement in biotechnological processes, several industrial wastes (organic and nutrient rich composition), have been exploited as a resource for the generation of value-added products such as bioactive compounds, biopolymers, biomaterials, biofuels, enzymes, biopesticides, bioplastics, and biohydrogen through microbial fermentation process.

A lignocellulosic material serves as a significant source for transformation into value added products (fine chemicals, delignification, nutraceutical, and enzymes). The process constitutes pretreatment of the wastes biomass, making of value-added products in fermenters and the recovery of end product. Pretreatment strategies can greatly increase the enzyme yields by several folds. Consolidation of new wide-ranging technologies for the organic waste exploitation will also stimulate the transition towards a circular economy. Therefore, viability and sustainability of the formation of new value-added products from bio-wastes and by-products streams will be discussed. The recent development and future prospects will discuss and challenges during the process will also be highlighted.

O-COB-03

Production of Gallic acid under solid-state fermentation by utilizing waste from food processing industries

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Abstract

Gallic acid (3,4,5-trihydroxybenzoic acid) is an industrially important organic acid that is found in plants as secondary metabolite. It possesses wide range of applications in healthcare, food and pharmaceutical industry, in manufacturing inks, paints, dyes and also in cinematography. The annual consumption of gallic acid in Pakistan is 8000 tons which is mainly met by importing this item from developed countries. This study was planned to assess the potential of various tannin rich bio-wastes [e.g., peels (banana, pomegranate, apple, and mango) and seeds (black plum, mango, apple, and tamarind)] from fruit processing industries to produce gallic acid by using Aspergillus niger via solid state fermentation. Different physical and chemical parameters were optimized to get the optimum yield of gallic acid. Among all bio-wastes, black plum seed powder gave highest yield of gallic acid i.e. 13.31 mg/g of substrate; the parameters being: substrate water ratio of 1:3, 72 hours of incubation period, 2 mL of inoculum, pH 5 and temperature of 30ºC. Carbon source supplementation i.e., glucose increased the synthesis of gallic acid to 14.5 mg/ g of substrate while addition of nitrogen sources had negative effect. Extraction of gallic acid was done by using Soxhlet extraction apparatus while FTIR was used for characterization. The solid state fermentation protocol for the production of gallic acid from tannin rich biowastes has been developed and proved to be cost-effective method. The results presented can be optimized further on large scale for industrial production of gallic acid.

Keywords: Gallic acid, Tannin rich, fruit waste, black plum seed, Aspergillus niger, solid state fermentation

O-COB-04

Synthesis and antioxidant screening of Novel indole amines

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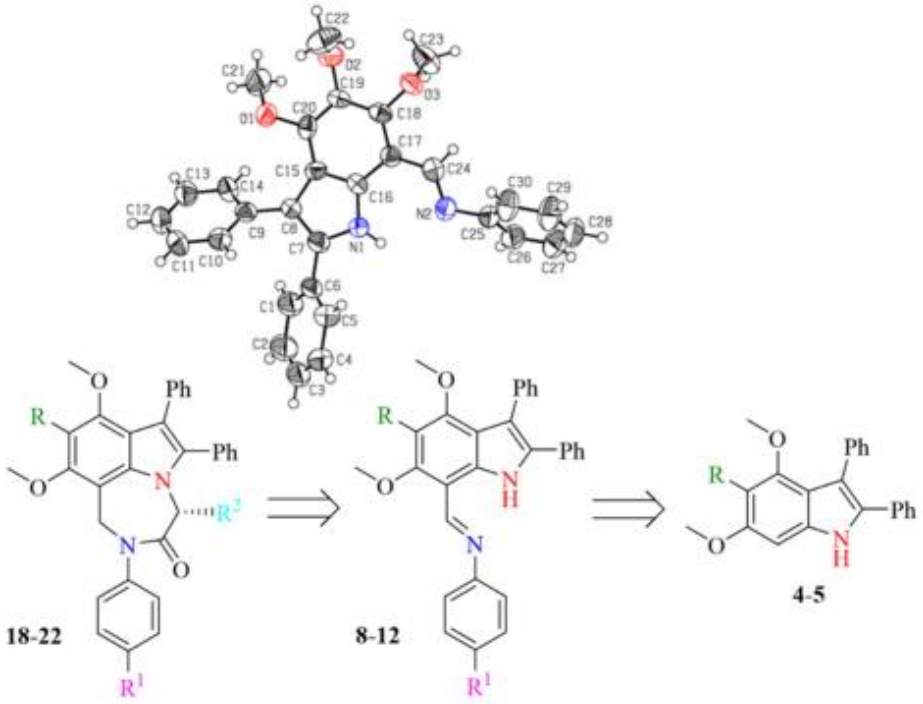
Abstract

Novel indoles amines have been synthesized and screened for antioxidant activity. Chiron approach is used to synthesis enantiopure heterocycles. Newly synthesized indole amines showed good antioxidant potential as compared to standard drugs. Novel indole amines **(**13–17**)** were synthesized and showed promising DPPH• scavenging activity, The H_2O_2 inhibition potential and the Ferric ion (Fe^{3+}) reducing antioxidant power assay. The pharmacological activity is tested by targeting indolic diazepines derivatives.



Keywords: Indoles, Indolic imines, Amines, Antioxidant activity

O-COB-05

Optimization and impact of different extraction parameters to extract phytochemicals from dried Phlomis stewartii leave's using Response surface methodology

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Abstract

Phlomis is genus of over 100 species in family Lamiaceae use to cope several diseases in living body. Phlomis stewartii is one of them found in desert area of Baluchistan (Pakistan). The plant was rarely evaluated in context of medicinal plant potential. Present worked aimed to evaluate yield of extract, phytochemical components, total phenolic contents (TPC) and total flavonoid contents (TFC) applying the Response surface methodology (RSM). RSM based on three independent variables and Box-Behnken design (BBD) was used for optimizing the extraction conditions, including solvent concentration, extraction time, and speed in range of (100 mL, 150 mL, 200 mL), (2 h, 6 h, 8 h), and (100 rpm, 150 rpm, 200 rpm) respectively, in addition to determine the trace bio-elements in Phlomis stewartii leaves. The highest results for response were observed under following condition: solvent concentration (200 mL), extraction time (8 h) and speed (150 rpm). The percentage of results was lowest for response on following condition such as solvent concentration (100 mL), extraction time (2 h), and speed (100 rpm). In conclusion, the outcome of this study clearly expressed that efficiency of extraction yield, TPC and TFC increase with increasing in duration of extraction time and greater solvent concentration, which results in better results. The data collected from this work should be useful to further develop and apply this plant source

O-COB-06

Improved bioavailability of Ebastine through development of transfersomal oral films

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Abstract

The main objective of this research work was the development and evaluation of transfersomes integrated oral films for the bioavailability enhancement of Ebastine (EBT) to treat allergic rhinitis. The flexible transfersomes, consisting of drug (EBT), lipid (Phosphatidylcholine), and edge activator (EA) Polyoxyethylene sorbitan monooleate or Sorbitan monolaurate, were prepared by conventional thin film hydration method. The developed transfersomes were further integrated into oral films using solvent casting method. Transfersomes were evaluated for their size distribution, surface charge, entrapment efficiency (EE %) and relative deformability. Whereas the formulated oral films were characterized for weight, thickness, pH, folding endurance, tensile strength, % elongation, mucoadhesion, degree of crystallinity, water content, content uniformity, in vitro drug release, ex-vivo permeation as well as in vivo pharmacokinetic and pharmacodynamics profile.The mean hydrodynamic diameter of transfersomes was detected to be 75.87 ± 0.55 nm with an average PDI and zeta potential of 0.089 ± 0.01 and 33.5 ± 0.39 mV respectively-. The highest deformability of transfersomes of 18.52 mg/sec was observed in VS-3 formulation. The average entrapment efficiency of the transfersomes was about 95.15 ± 1.4 %. Transfersomal oral films were found to be smooth with an average weight, thickness and tensile strength of 174.72 ± 2.3 mg, 0.313 ± 0.03 mm, and 36.4 ± 1.1 MPa respectively. The folding endurance measured to be 132 ± 1 with a pH and elongation of 6.8 ± 0.2 and 10.03 ± 0.4 % respectively. The ex vivo permeability of EBT from formulation ETF-5 was found approximately 2.86 folds higher than the pure drug and 1.81 folds higher than plain film (i.e., without loaded transfersomes). The relative oral bioavailability of ETF-5 was 2.95 and 1.7 folds higher than that of EBT-suspension and plain film respectively. Also, ETF-5 suppressed the wheal and flare completely within 24 h. Based on the physicochemical considerations as well as in vitro and in vivo characterizations, it is concluded that the highly flexible transfersomal oral films (TOFs) effectively improved the bioavailability and antihistamine activity of EBT.

Keywords: Bioavailability, Ebastine, Edge activator, In vivo, Phospholipids, Transfersomes

O-COB-07

Designed synthesis of thiobarbituric acid hybrid structures as potent urease inhibitors

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Abstract

A series of thiobarbiturates 4a–4e synthesized by condensing 1,3-diethylthiobarbituric acid 3 with a variety of aromatic aldehydes with varied structural features and substitution at active methylene position of thiobarbituric acid. Afterward, thiobarbituric acid structures were characterized through FT-IR, NMR spectroscopy and mass spectrometry. Subsequently, the inhibitory potential of thiobarbiturates 4a–4e against urease enzyme was evaluated. The inhibitory potential of all synthesized analogues in terms of IC50 value was observed in the range of 22.53 ± 0.76 to 79.34 ± 0.52 μM by comparing with thiourea (IC50 21.25 ± 0.15 μM) as a standard urease inhibitor. Most of the analogues exhibited potent inhibitory activity against urease. After interesting findings, structure activity relationship (SAR) has been established for all analogues. Docking studies revealed that synthesized analogues interacted with active site residues
of bimetallic nickel center of the urease enzyme through, thiolate, π-π stacking and hydrogen bonding interactions.

O-COB-08

Solubilization study of metal fluoride complexes of nickel, cobalt and copper in anionic micellar media by conductometric and spectroscopic techniques

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Abstract

Micellization is an interesting property of surfactants mimic to biological membranes which make surfactants viable for biological and pharmaceutical studies. So, the micellar solubilization is a useful tool to investigate the interaction of various bioactive agents in biological systems. This study was aimed to evaluate the solubilization of the metal complexes of Nickel, Cobalt and Copper with nitrogen donor ligands such as [Ni(dmen)2F2].8H2O, [Ni(phen)3]F2.EtOH.MeOH.8H2O, [Co(phen)3]F2·2H2O and [Cu(im)6]F2·4H2O. The anionic surfactants sodium stearate (SS) and sodium dodecyl sulfate (SDS) were found to be a suitable micellar system for their solubilization study. The variation in CMC at various temperatures (298K, 308K, 318K and 328K) was investigated by specific conductivity measurements. The conductivity measurements were used to calculate the micellization parameters such as degree of dissociation, Gibb's free energy of micellization (ΔGm), entropy of micellization (ΔSm) and enthalpy of micellization (ΔHm). These parameters revealed that the phenomenon of micellization is entropy driven and spontaneous due to the more negative value of (ΔGm). UV-Vis spectroscopy study was carried out to uncover the interaction and partitioning of complexes in micellar media of SS and SDS. The partition coefficient, binding coefficient, energy of partition, and binding energy were determined and results showed that the complexes portioned in the micellar media of SDS and SS and reside at the inner side of micelles near the hydrophilic shell of micelles. The biological potential of the complexes was also explored by antioxidant assay, hemolytic assay and cytotoxicity assay. Hence, the micellar solubilization model could be a quantitative understanding to design a true solubilization model to transport the metal-based dugs at specific site across plasma membrane in the micelle-based drug delivery systems.

Keywords: Meta complexes, Micellar solubilization, Electrical conductivity, UV–Visible spectroscopy, anionic surfactants

O-COB-09

A greener approach towards peptoid modification chemistry

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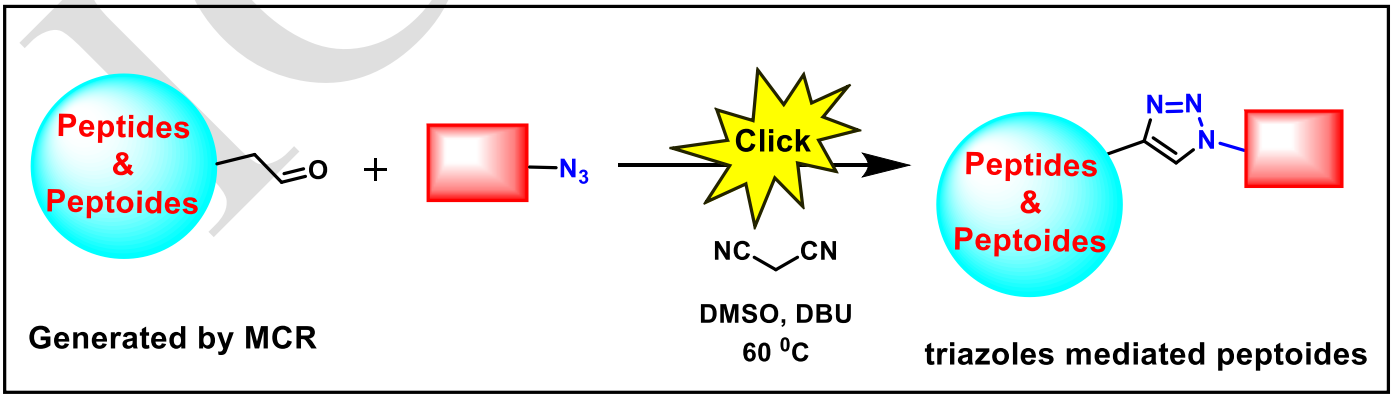
Abstract

A new greener and highly regioselective formation of peptoid-functionalized 1,4-disubstituted-1,2,3-triazoles is described by merging the Ugi-4CR and metal-free click reactions. The MCR generated peptoids with the insertion of a varity of natural carboxylic acids, as well as synthetic peptides. Furthermore, modified lipids and monofunctional polyethylene glycols have also been utilized as substrates for this protocol. Finally, the aldehyde moiety presented at the peptoid framework reacted with malononitrile to generate *in-situ* alkylidene malononitriles, which act as dipolarophiles in the presence of DBU in the 1,3-dipolar cycloaddition reaction in a metal-free condition for the generation of complex peptidomimetic products.

Keywords: Metal-free, Cycloaddition reaction, Ugi-4CR, Highly regioselectivity, Peptoids



O-COB-10

Chitosan nanoparticles coated with curcumin as seed priming agents induce stress tolerance in wheat (*Triticum aestivum* L.) for sustainable growth

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Abstract

The germination, growth and development of wheat have greatly been affected by the ecotoxicological conditions and environmental stresses over the last few decades. The abiotic stresses induce negative impacts on metabolic processes, biochemical and physiological attributes. Consequently, the disturbed cellular pathways and disrupted metabolic functions inhibit plant growth and limit crop productivity. Over the last few years, chitosan nanoparticles (CNPs) have shown promising applications in agriculture. Seed priming significantly increases the peroxidase, protease, non-reducing sugars, CMS and relative water content in seedlings under normal and stress conditions. Considering the plant growth-promoting, immunomodulator and non-hazardous nature of chitosan and antioxidant potential of curcumin we prepared CNPs coated with curcumin as ecofriendly priming agents for wheat seeds. The effects of aforesaid priming agents will be discussed on biochemical attributes under normal and stress conditions. The priming effects on hydrolytic enzymes, important biomolecules, enzymatic and non-enzymatic anti-oxidants will be discussed on primed, hydro-primed and non-primed control seeds. Further, the stress emulating-role of aforesaid eco-friendly priming agents will be discussed on biochemical attributes of wheat seedlings originated from primed, non-primed and controlled seeds under normal and stress conditions.

Keywords: Seed programming, Seed pre-conditioning, MDA, nano-priming, sustainable agriculture

O-COB-11

Mutagenicity, cytotoxic and antioxidant activities of Ricinus communis different parts

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Abstract

Ricinus communis (castor plant) is a potent medicinal plant, which is commonly used in the treatment of various ailments. The present study was conducted to appraise the cytotoxicity and mutagenicity of Ricinus communis along with antioxidant and antimicrobial activities. Cytotoxicity was evaluated by hemolytic and brine shrimp assays, whereas Ames test (TA98 and TA100) were used for mutagenicity evaluation. Plant different parts were extracted in methanol by shaking, sonication and soxhlet extraction methods. The Ricinus communis methanolic extracts showed promising antioxidant activity evaluated as through total phenolic contents (TPC), total flavonoid content (TFC), DPPH free radical inhibition, reducing power and inhibition of linoleic acid oxidation. Ricinus communis seeds, stem, leaves, fruit and root methanolic extracts showed mild to moderate cytotoxicity against red blood cells (RBCs) of human and bovine. Brine shrimp lethality also revealed the cytotoxic nature of extracts with LC50 in the range of 0.22-3.70 (µg/mL) (shaking), 1.59-60.92 (µg/mL) (sonication) and 0.72-33.60 (µg/mL) (soxhlet), whereas LC 90

values were in the range of 345.42-1695.81 µg/mL, 660.50- 14794.40 µg/mL and 641.62-15047.80 µg/mL for shaking, sonication and Soxhlet extraction methods, respectively. Ricinus communis methanolic extracts revealed mild mutagenicity against TA98 (range 1975±67-2628±79 revertant colonies) and TA100 (range 2773±92-3461±147 revertant colonies) strains and these values were 3267±278 and 4720±346 revertant colonies in case of TA98 and TA100 positive controls, respectively. Ricinus communis methanolic extracts prevented the H2O2 and UV to Plasmid pBR322 DNA oxidative damage. Results revealed that Ricinus communis is a potential source of bioactive compounds and in future studies the bioactive compounds will be identified by advanced spectroscopic techniques.

Keywords: Medicinal plant, Extraction techniques, Antioxidant, DNA induced damage, Bioassays

O-COB-12

Exploration of recombinant papase as a new strategy to combat Dengue virus

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Abstract

The present study explores potential of Carica papaya phytochemicals and papase as anti- dengue agent. C. papaya leaves have shown promising results in cure of dengue fever in some initial trials but the true mechanism still remains unclear. Therefore, the study aimed to find potential of different phytochemicals and papain protein to cure dengue. Methanolic extracts of leaves promising antioxidant activity through DPPH and linoleic acid scavenging activity. The extracts showed efficient activity against selected microbial strains. Principal compounds in C. papaya were evaluated through molecular docking of C. papaya novel bioactive compounds against DENV NS2/NS3 serine protease established important role of 9 compounds against these proteins. Three compounds, epigallocatchin, baicalein and fisetin showed high interaction with His51, Asp75, Ser135 of serine protease of dengue virus. Genetically engineered papase gene was heterologously expressed in E. coli BL21 through pET102TOPO/D which showed hyperexpression of papase serine protease activity upto 3 h induction with IPTG as 16.2± 1.05 u/mL. The administration of recombinant protein+CPE at different levels increased platelet count, leucocyte count, granulocytes, eosinophil count and lymphocytes, red blood cell count, hemoglobin, blood glucose level, haematocrit and mast cell count. all the parameters. The study also established that combination of recombinant papase with plant leaf extracts showed synergetic effect on eradication of dengue in mice by interfering with NS2B and NS3B proteins of virus through its serine protease activity for eradication of dengue.

Keywords: Papain, gene cloning and engineering, anti-microbial, DPPH, expression, anti-dengue effect

O-COB-13

Enzyme catalyzed synthesis of new and bioactive molecules

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Abstract

Biotransformation is an efficient tool for carrying out reactions at otherwise inaccessible sites in the molecules with high stereo- and regioselectivity. The specific nature of enzymes make this technique a productive method for the production of enantiomerically pure chemicals, rendering the method one of the choices for drug development. Microbial enzymes have been utilized for the transformation of a variety of skeletons. During this study we have investigated the microbial transformation of various drugs and compared the results with their metabolism inside the animal body, reported previously. In most of the cases it was found that the compounds under study produced similar metabolites which were obtained from in vivo metabolism. Some of these products were found to be new and others exhibited good biological potential as well.

O-COB-14

Grewia asiatica juice supplementation exhibits anti-amnesic effects via modulation of cholinesterases and redox imbalance in the brains of scopolamine-amnesic Sprague Dawley rats

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Abstract

Grewia asiatica L. fruit natively called phalsa is a popular berry of Pakistan and widely consumed in the form of fresh juices and carbonated drinks in the summer season. The berry is enriched with antioxidants such as phenols, flavonoids, anthocyanins, and vitamin C. Scientifically, it is the least explored berry in terms of neuromodulatory activities, and therefore, in the designed study, chronically fed rats with the different dilutions (5%−30%) of fruit juice were subjected to behavioral assessment for anxiety, depression, and cognition (spatial memory) followed by biochemical analysis of isolated brains. Results revealed a prominent impact of 20 and 30% dilutions of fruit exudate as treated animals showed anxiolytic behavior to central zone (P < 0.05) of open field test (OFT) and open arms of elevated plus maze (EPM) (P < 0.05) in anxiety models. Overall, immobility of rats treated with a higher concentration of exudate in forced swim test (FST) was reduced (P < 0.05) presenting antidepressant-like activity. Moreover, in learning and memory experimental models, the treated animals reversed scopolamine-induced amnesic effects as evident from improved step-through latencies (P < 0.05 vs. scopolamine; passive avoidance test), spontaneous alternation behavior (P < 0.05 vs. scopolamine; Y-maze test), discrimination index (P < 0.05 vs. scopolamine; novel object recognition test), and escape latencies (P < 0.05 vs. scopolamine; Morris water maze). Biochemical studies of isolated brains from treated rats demonstrated significantly elevated levels of superoxide dismutase and glutathione peroxidase (P < 0.05), whereas levels of acetylcholinesterase and malondialdehyde level (P < 0.05) were reduced, indicating its potential to reduce oxidative damage in the brain and modulation with the cholinergic system. The outcomes of studies support the benefits of phytoconstituents possessed by G. asiatica fruit in the amelioration of neurological disorders that could be due to their antioxidative capacity or due to interaction with GABAergic, serotonergic, and cholinergic systems in the brain.

O-COB-15

Dyes Adsorption By Hydroxyethyl Cellulose Grafted With Copolymer Of Polyaniline And Polypyrrole

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Abstract

Preparation of Hydroxyethyl cellulose (HEC) grafted with copolymer of polyaniline (PANI) and polypyrrole (PPy) (HEC/PANI-PPy) was carried out and used for the adsorption of methyl Orange (MO) and Rhodamine B (RB). Biopolymer (HEC/PANI-PPy) was characterized by Fourier transform infrared (FT-IR) Scanning electron microscope (SEM) Powder X-ray diffraction (XRD) Brunauer-Emmett-Teller (BET). Dyes adsorption data was evaluated with different isotherm models, best fitted model for this research is Langmuir Isotherm and was found that adsorbent could be excellent alternative for the removal of dyes from textile wastewater.

O-COB-16

Synthesis and biological evaluation of novel ciprofloxacin derivatives as potential antitumor agents

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Abstract

Ciprofloxacin is a second generation of synthetic fluoroquinolones and was first patented in 1983. It was approved as an antibiotic for clinical use by FDA (USA) in 1987. Since then it is the most widely prescribed fluoroquinolone throughout the world in respiratory, skin, bone, and joint infections. It also displays anti-proliferative as well as

apoptotic activities against a number of cancerous cells. These studies have led us to synthesize novel structural hybrids of ciprofloxacin linked with a variety of anilides and oxadiazoles. Moreover, carboxamide and sulfonamide derivatives of ciprofloxacin were also synthesized. After that antitumor activity of these derivatives was assessed against liver and breast cancer cell lines (Huh-7 and MCF-7, respectively) using MTT assay. Among ciprofloxacin-based anilide series, methyl 1-cyclopropyl- 6-fluoro-4-oxo-7-(4-(2-oxo-2-(phenylamino)ethyl)piperazin-1-yl)-1,4-dihydroquinoline-3- carboxylate inhibited the growth of tumor cells by displaying 68.36% cell viability at 100 µg/mL concentration. In ciprofloxacin-oxadiazole hybrids, methyl 1-cyclopropyl-6-fluoro-4-oxo-7-(4-(2- ((5-(phenoxymethyl)-1,3,4-oxadiazol-2-yl)thio)acetyl)piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylate depicted comparatively lower cell viability value (81.91% using 100 µg/mL concentration) than the other compounds. Similarly, primary screening of carboxamide and sulfonamide series revealed methyl 1-cyclopropyl 7-(4-(2-bromoacetyl)piperazin-1-yl) 6-fluoro- 4-oxo 1,4-dihydroquinoline-3-carboxylate, a promising lead compound with cell viability of 42.66% at 100 µg/mL concentration. These representative compounds were then in-silico modeled to delineate the potential mechanistic insights for their anti-proliferative activity. Strong inhibition of topoisomerase II with higher binding affinity highlighted the importance of structural hybrids of ciprofloxacin which can be helpful in the near future to develop potent anticancer agents.

O-COB-17

Bio-surfactant is a potent tool for the Bioremediation of heavy metals and organic compound in contaminated soil and water

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Abstract

Environmental pollution has a negative impact on human health. According to the revolution of industries, many hazardous health problems are caused by the consumption of contaminants and chemicals in large amounts in industries. Bioremediation has evolved as an active method for minimizing the adverse effects of pollution and making polluted soil-less contaminated and free of dangerous or undesired compounds, and it has been shown to be a relatively cost-effective option. In bioremediation methods, the microbial population consumes heavy metals and toxins as food. People are becoming more aware of microbial bioremediation of pollutants as they seek to remediate toxins in the environment via the use of trustworthy approaches. The bioremediation process uses microorganisms due to their ability to degrade pollutants from different environments by using their metabolism via biochemical pathways associated with the growth and other organismic activities. Altered microorganisms are capable to degrade hazardous substances present in polluted environments into harmless end-products. External genes are introduced into the genomes of genetically modified microorganisms (GEMs), which can be isolated using recombinant DNA technology from the same or distinct organisms of the same species. These Genetically engineered microbes are used to attain proficient strains for bioremediation of polluted environments by having improved ability to degrade a variety of waste products. Heterologous proteins, which have developed as a unique and cost-effective approach for the bioremediation of a range of organic and inorganic pollutants, are visible on the cell surface. Microbes must increase their catabolic activities by genetic modification, the introduction of specific enzymes, and the development of selective characteristics in order to refurbish the target molecules during active biodegradation.

Keywords: Organic compounds, Soil water, phytoremediation, genetically modified microbes, biodegradation.

O-COB-17

Single Nucleotide Polymorphism analysis of APOA5 Gene In HypertriglyceridemiC Patients

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Abstract

Hypertriglyceridemia is the characteristic of various metabolic disorders and causative factors include high plasma triglyceride level, genetic and other secondary reasons. Among various human populations, specific SNP (single nucleotide polymorphism) of APOA5 gene correlated with plasma triglyceride levels. The proposed study was intended to associate APOA5 SNPs with hypertriglyceridemic patients of Pakistan and response of fibrate therapy to hypertriglyceridemic patients by observing their selected gene SNPs with risk allele for disease. For this purpose, blood sample of 50 patients were collected for DNA extraction by standard inorganic method. Extracted DNA was analyzed biochemically and genetically following selection and genotyping of APOA5 gene in order to know SNP variants with risk alleles. Data analysis and statistics based calculations were accomplished by SPSS. Lipid profile including TG (triglyceride), HDL (high density lipoprotein) and LDL (low density lipoprotein) levels of hypertriglyceridemic patients was analyzed, and then compared it to normal and fibrate treated individuals. Fibrate decreased TG level and LDL about 30-45% and 20-25% respectively; increased high density lipoprotein about 10-15% and total cholesterol was decreased about 6-8% in Pakistani population. One tagging APOA5 (rs662799) SNP in 50 hypertriglyceridemic patients with high plasma triglyceride levels was analyzed. Hypertriglyceridemia risk was significantly increased by minor allele of APOA5 rs662799 polymorphism. Minor allele carriers of rs662799 had odds ratio of (95% CI) 1.5 (1.03-2.18) (P = 0.032). Risk allele frequency was different among hypertriglyceridemic patients, healthy controls and fibrate treated hypertriglyceridemic individuals. Our results showed that 87.5% of healthy controls exhibited no risk allele while 78% did not show this risk allele among hypertriglyceridemic patients.

Parallel Session III: Analytical, Inorganic & Physical Chemistry

O-AIP01

Kinetic and thermodynamic study of Acid Red 1 removal by biocomposites

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Abstract

Novel eco-friendly and economically favorable chemically modified biosorbents and biocomposites from sugarcane bagasse (SB) have been investigated for the first time for efficient removal of Acid red 1 dye from wastewater. Fabricated biosorbents and biocomposites were characterized analytically. Batch adsorption experiments have been performed to optimize operating parameters and the determined optimum conditions are; pH: 2, dose: 0.05 g, contact time: between 60–75 min, initial dye concentration: 400 mg/L, and temperature: 30 o C, at which maximum Acid red 1 dye removal capacities were found (within range of 143.4–205.1 mg/g) by as-designed SB-derived chemically modified biosorbents and biocomposites. This high adsorption capacity was accompanied due to its large specific surface area (30.19 m^2/g) and excessive functional active binding sites. In terms of the nature of adsorption process, kinetic and isothermal studies demonstrated that experimental data shows greater fitness with pseudo 2 nd order and Langmuir model. Thermodynamics analysis revealed that the adsorption process is spontaneous, feasible, and exothermic in nature. Adsorption selective studies signify that lower concentration of co-existing metallic ions were not interfered during the removal of Acid red 1 dye, which confirms that under optimized adsorption conditions the biosorbents and biocomposites exhibited greater affinity for dye molecules. Hence, it is anticipated that this type of novel SB-derived biocomposites could be considered as greener potential candidate material for commercial scale dye removal applications from industrial wastewater.

O-AIP02

Micellar Enhanced Flocculation for removal of pollutants from synthetic wastewater

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Abstract

Surfactant-based removal of reactive yellow 160 (RY-160) from synthetic waste water has been reported in this research work. Micellar enhanced flocculation technique was applied and optimized for the said purpose. The mixture of anionic surfactants, obtained from a bio-degradable source (base soap), has been found to have great potential to solubilize dye molecules. The polyvalent salts are able to flocculate the micelles and help in their subsequent removal. The removal of dye was analyzed using UV/Visible spectrophotometer. Different factors such as the effect of change in concentration, pH, temperature, contact time, and electrolyte were studied to evaluate the adsorption characteristics and removal efficiency of the process. The data obtained was further used to study the mechanism of adsorption with the help of various models e.g., Langmuir, Freundlich, Temkin, and Dubinin–Radushkevich (D-R). The kinetic parameters were also calculated by employing pseudo-1 st and pseudo-2 nd order kinetic models. Furthermore, thermodynamic calculations were performed to determine the change in Gibb's free energy (ΔG^o), enthalpy (ΔH^o), and entropy (ΔS^o). The results make it evident that the micellar flocculation-based adsorptive removal is an excellent and sustainable approach for the treatment of wastewater.

Keywords: Surfactants, flocculation, adsorption, isotherm, thermodynamics

O-AIP03

Optimized production of biodiesel from non-edible (Tamarindus indica) seed oil

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Abstract

Biodiesel is a clean burning non-petroleum-based diesel fuel and has received dire attention over the past decade as an alternative to fossil fuels. Due to favorable characteristics, biodiesel is now widely accepted as a viable alternative to petroleum-derived diesel fuel. However, the higher production costs, which are largely due to the use of expensive food-grade vegetable oils as raw materials, is a major obstacle to its economic viability. The current study aims to scrutinize the potential of Tamarindus indica seed oil for biodiesel synthesis through alkali-catalyzed transesterification. Output parameters such as the molar ratio of alcohol to oil, the amount of catalyst, and reaction time were optimized by using Taguchi method. The fatty acid contents of both oil and biodiesel were determined by GC. The optimal conditions for obtaining 93.5% biodiesel were found to be a 6:1 alcohol to oil molar ratio, 1.5% wt/wt catalyst, and 2 h reaction time. The 'molar ratio of alcohol to oil' (75.9%) had the highest % contribution, followed by the amount of catalyst (20.7%). The major fuel properties of Tamarindus methyl esters formed under ideal conditions were found to be within the defined limits of ASTM D6751 for biodiesel, suggesting that it could be used as a potential petro diesel substitute.

O-AIP04

Stoichiometricarchitectural impact on thermomechanical and morphological behavior of segmented Polyurethane elastomers

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Abstract

Segmented polyurethane elastomers are extensively used in various applications as a consequence of supple and superior performance. Nevertheless, researchers pay close attention on the design and synthesis of segmented polyurethane elastomers through the well- organized laboratory process. To investigate the properties of synthesized modifier based on chemical structure, firstly each kind of unknown structure and composition ratio of TPUs was determined by using a new method. Four series of linear polyurethane elastomers, each comprised of seven samples are synthesized using hydroxyl terminated polybutadiene as macrodiol, toluene diisocyanate and four different chain extenders: 1, 2 Ethane diol; 1, 4 Butane diol; 1, 6 Hexane diol and 1, 8 Octane diol. The functional linkages for the

development of polymers have been confirmed via Fourier transform infrared spectroscopy. Hydrogen bonding index calculated from vibrational modes of C=O group are obtained in the range of 1.08–1.394. The thermal stability is observed up to 290 °C by thermal gravimetric analysis. Swelling behavior showed 50% of industrial waste water uptake. The true tensile strength is observed up to 8.48 MPa with 1,4 butane diol as chain extender. The secant modulus at 1% strain rate is found in the range of 0.30 to 12 MPA. The maximum value of toughness is observed as 3.26 J-mm^{-2} for 1,4 butane diol chain extenders. Scanning electron microscopic analysis has revealed morphological phase segmentation based on composition.

O-AIP05

Development of Bi_2O_3-ZnO heterostructure for enhanced photodegradation of rhodamine B and reactive yellow dyes

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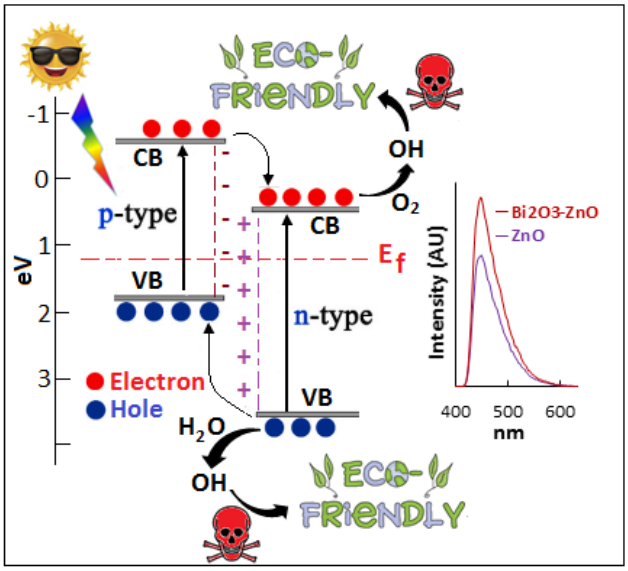
Abstract

Semiconductor based photocatalysis is one of the effective techniques of AOPs for environmental remediation. In present work, the development of an efficient photocatalyst formed by coupling of p-type Bi_2O_3 and n-type ZnO is reported. The Bi_2O_3-ZnO heterostructures with 5, 10 and 15% Bi_2O_3 were synthesized by co-precipitation method. The prepared heterostructures were characterized by various advanced techniques including XRD, XPS, UV-Visible spectroscopy, FTIR, SEM and surface area measurement. The prepared ZnO and Bi_2O_3-ZnO heterostructures were tested as photocatalysts for photodegradation of dyes using mixed solution of rhodamine B and reactive yellow dyes. The 5% Bi_2O_3-ZnO heterostructure was found as most efficient photocatalyst with 93 and 91% photodegradation of rhodamine B and reactive yellow dyes, respectively. It was found that incorporation of 5% Bi_2O_3 with ZnO enhanced the photocatalytic activity about 15 times towards photodegradation of dyes.



Mechanism of photodegradation of dyes

O-AIP06

Optimum conditions for the removal of Rhodamine B from aqueous system by Micellar Enhanced Ultrafiltration

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Abstract

Micellar enhanced ultrafiltration (MEUF) has proved itself to be a potentially attractive tool to remove contaminants from waste water. The reported study is particularly focused on the removal of Rhodamine B dye using micellar solution of anionic surfactants, i.e., Sodium dodecyl sulfate (SDS) and Sodium Oleate (SO). Removal efficiency has been assessed in terms of rejection percentage and permeate flux, using cellulose membrane of 10,000 molecular weight cut off (MWCO). The effects of various factors, i.e., ionic strength, concetaqntration of surfactants, concentration of electrolyte, pH, operating pressure and rotations per minute (RPM) has been observed. The maximum rejection has been observed and overall, it has been observed that the rejection coefficient is higher at higher concentration of surfactants and electrolyte and at lower values of pH, RPM and transmembrane pressure.

O-AIP07

Investigation of photo-esterification capability of RGO/BiVO 4 for the production of biodiesel from soapnut oil and its computation study

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Abstract

Non-edible feedstocks are economically viable for the production of biodiesel but presence of higher amount of free fatty acids (FFAs) in these oils is a main hurdle for getting good quality biodiesel. This issue can be resolved through esterification prior to transesterification of oil. This work was designed to evaluate the catalytic activity of two sunlight active photocatalysts; BiVO4 and RGO/BiVO4 for the esterification of higher FFA content present in soapnut oil. These catalysts were characterized through SEM, XRD and FT-IR. Experimental results revealed that RGO/BiVO4 exhibited higher catalytic activity as compare to BiVO4 for the esterification of FFA under sunlight irradiation. Different process variables were optimized and maximum conversion of FFA (88 %) was obtained at 3:01 methanol to oil ratio, 5 % catalyst dose, 300 rpm stirring speed and 3 h of reaction time. Esterified oil was than transesterified by using MgO-KOH heterogeneous catalyst. The physic-chemical analysis of synthesized biodiesel revealed that it meets ASTM standards. Mechanistic study of photo-esterification reaction was conducted by using density functional theory (DFT) method which revealed that the photo-catalyst reduced the energy barrier of activation from 51.67 kcal/mol to 0.7495 kcal/mol. It was concluded that the photo-catalysts act as efficient catalysts with higher capability of esterification of non-edible oil. This project also provided reliable basic theoretical data for the understanding of photo-esterification mechanisms.

O-AIP08

Patterns of essential/toxic metals distribution in the blood of diabetes mellitus patients in comparison with healthy donors

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Abstract

Diabetes mellitus is growing in prevalence worldwide. It is a serious disease which occurs when human body has difficulty in properly regulating the amount of glucose in your blood. This study was conducted to evaluate the essential/trace metals in the blood of diabetes mellitus patients in comparison with healthy donors. Selected essential/toxic metals (Fe, Ca, Zn, Cr, Cd, Se, Pb, V and Sr) were measured in the blood of diabetes mellitus patients and counter-part healthy donors by atomic absorption spectrometry employing nitric acidic acid-perchloric acid based wet digestion. The mean concentration of Cd, Pb, Fe and V were found to be significantly higher in the blood of diabetes mellitus patients compared with the healthy donor however significantly higher concentration of Zn, Se, Cr, and Ca were observed in the healthy donors. Most if the metal levels revealed higher dispersion and asymmetry in the blood of the patient than the healthy donors. The correlation study revealed significantly diverse relationship among the metals in the patients and healthy donors. Thee multivariate apportionment of the metals in the blood of

the patients and healthy donors was also significantly different. The study evidenced considerably divergent variations in the metal levels in diabetes mellitus patients in comparison with healthy donors.

Keywords: Metals; Diabetes; Blood; AAS; Statistical Analysis; Pakistan

O-AIP09

Investigation of Cu-doped Zinc Oxide Zn1-xCuxO (x = 0.01, 0.02, 0.03, 0.04, 0.05) based nanostructures for the elimination of Methylene Blue dye pollutant under sunlight

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Abstract

Herein, copper (Cu) doped zinc oxide (ZnO) namely Zn 1-x Cu x O (x = 0.01, 0.02, 0.03, 0.04, 0.05) are grown by hydrothermal method for photo catalytic activity. The grown samples were characterized with XRD, FTIR, SEM, UV-vis. The XRD results confirmed the successful doping of Cu ions without altering basic hexagonal structure of ZnO. FTIR results also confirm the presence of metal-oxygen bonds vibration related to Zn-O bonds. UV-vis results showed that the energy band gap decreased with the increase in the doping concentration of Cu. SEM images shows the nano rods type morphology which is improved with the increasing Cu doping. Photocatalytic activities of all synthesized samples were tested against methylene blue (MB) dye under the sunlight irradiation. The Zn 0.95 Cu 0.05 O photo catalyst show a best photo catalytic activity with 99.9% elimination of MB dye within 60 min, as related to the pure ZnO and 1%, 2%, 3%, and 4% Cu doped ZnO. In comparison to the other catalyst, value of the rate constant for Zn 0.95 Cu 0.05 O was greater than the pure catalysts. The excellent photocatalytic activity of Zn 0.95 C 0.05 O is accredited to 1) presence Cu ions that successfully suppress high recombination of electron hole pair which, in turns find the enough time to produce extra reactive species for degradation MB dye and 2) Lower energy bandgap of ZnO by 5% Cu doping in visible region which leads to higher number of electrons excitation from valence band to conduction band. Hence, the present finding introduces a strategy to reduce the energy bandgap of ZnO from UV

O-AIP10

Improvement of activity, thermo-stability and fruit juice clarification characteristics of fungal exo-polygalacturonase

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Abstract

An extracellular exo-polygalacturonase (exo-PG) from Penicillium notatum was immobilized in sodium-alginate matrix through two different protocols, viz. covalent bonding and adsorption to enhance its catalytic activity, thermal stability and life-time properties for industrial applications. Covalent immobilization was more efficient in terms of high relative activity (45.89%) and immobilization yield (71.6%) as compared to adsorption. Immobilized exo-PG derivatives displayed maximum activities at pH 5.5 and55 °C as compared to free enzyme which showed its optimum activity at pH 6.0 and 50 °C. The affinity of enzyme towards its substrate (K m) was reduced after immobilization and Vmax of covalently immobilized exo-PG decreased to 66.7% while the V max value of adsorbed enzyme increased up to 150% as compared to free counterpart. Both immobilization techniques greatly enhanced the thermal stability profile of the enzyme. At 60 °C, immobilized exo-PGs retained more than 90% of their residual activities after 60 min of heating, while free enzyme did not show any activity at the same temperature. Thermodynamic properties (i.e., Ea, ΔH*, ΔS*and ΔG*) of the free and immobilized enzymes were also investigated. Sodium-alginate covalently immobilized and adsorbed enzymes showed excellent recycling efficiencies and retained 50.0% and 41.0% of original activities, respectively after seven consecutive batch reactions. Moreover, the immobilized enzymes treatment achieved promising results in turbidity and viscosity reduction as well as clarity amelioration in

various fruit juices. Altogether catalytic, thermo-stability and fruit juices clarification characteristics of the immobilized exo-PGs suggest a high potential for biotechnological exploitability

O-AIP10

Storage effect in the levels of aflatoxins in selected edible seeds samples from, central cities of Punjab, Pakistan

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Abstract

Five twenty (520) samples of edible seeds and 520 samples of edible oilseeds (sunflower, Palm, peanuts, sesame, cotton, & Grapeseed) were gathered from markets, superstores (2-years storage and 6-months storage period) from the central cities of Punjab, Pakistan. The natural occurrence of aflatoxins (AFs) was investigated using HPLC. The outcomes have exposed that 127 (48.8%) samples of 2-years storage period and 125 (48.08%) samples of 6-months storage period edible seeds were observed to be contaminated with AFs. The maximum average amount of AFB 1 and total AFs in 2-years storage period seeds were 28.6 ± 4.5 and 51.3 ± 10.4µg/kg, respectively. The 127 (48.8%) samples of 2-year storage and 125 (48.08%) samples of 6-months storage period edible oils were positive with AFs. The maximum average amount of AFB 1 (22.4 ±8.5 µg/kg) and total AFs (25.3 ± 9.2 µg/kg were documented in 2-years storage period oil samples, and the amount of 11.9 ± 3.2 and 13.7 ± 3.9 µg/kg were documented in sunflower oil samples, respectively. The results have documented a significant difference in total AFs levels in edible seeds & oil samples available ($\alpha = 0.05$ & 0.01).

Keywords: storage; aflatoxins; edible seeds; oil; HPLC

O-AIP11

Water splitting: design strategies (selected examples) challenges and way forward

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Abstract

Solar-driven water splitting is deemed a viable option to produce sustainable hydrogen. One straightforward approach is to employ particulate photocatalytic systems, that retain their intrinsic activity and are competitive with fossil-fuel-derived hydrogen on a levelized cost basis. However, all the powder-based solar water-splitting systems tested thus far fall short on account of hydrogen production efficiency values required for practical applications. Functionally, in a typical particulate photocatalytic system, involves three key steps: (i) charge generation, (ii) charge trapping, interfacial electron exchange and (iii) subsequent surface chemical reaction that control the process efficiency. In the context of particulate photocatalysis, this work describes the photocatalytic properties and applications of semiconducting layered framework carbon nitride and selected nano metal oxides materials. Furthermore, by exploiting the band alignment strategy, the construction of carbon nitride isotype (type II) semiconductor heterojunctions and redox mediation to shuttle charges in metal oxides with the aim of suppressing the exciton recombination for the successful initiation of desirable redox processes (HCO2H, water splitting) are presented.

O-AIP12

Evaluation of Bis-(2-ethylhexyl) phthalate from Lactobacillus plantarum BCH-1 by using GC-MS and ESI-MS/MS

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Abstract

Bis-(2-ethylhexyl) phthalate has been reported as a potent bioactive secondary metabolite, naturally produced by bacterial, fungal, and algal species. In the current work, various analytical techniques were used for the detection and evaluation of Bis-(2-ethylhexyl) phthalate (BEHP) from Lactobacillus plantarum BCH-1. Bioactive compounds were extracted by ethyl acetate and BEHP was fractionated by gradient column chromatography from crude extract. Based on FT-IR followed by GC-MS and ESI-MS/MS, compound was identified to be Bis-(2-ethylhexyl) phthalate (BEHP). The antibacterial activity of purified compound was determined by disk diffusion assay by observing inhibition zone against Escherichia coli (12.33±0.56mm) and Staphylococcus aureus (5.66±1.00mm). Besides, antilarval activity was performed against Culex quinquefasciatus Say larvae and noted that BEHP showed 100% mortality after 72 h at the concentration of 250ppm. After 72h, inhibitory effect of acetylcholinesterase was detected as 29.00, 40.33, 53.00, 64.00, and 75.33 (%) at 50, 100, 150, 200, and 250ppm, respectively. In the comet assay, mean comet tail length (14.18±0.28µm), tail DNA percent damage (18.23±0.06%), tail movement (14.68 ± 0.56 µm), Comet length (20.62± 0.64µm), head length (23.75± 0.27 µm), and head DNA percentage (39.19 ± 0.92 %) were observed at 250 ppm as compared to control. Conclusively, the resultant compound, BEHP from L. plantarum BCH-1 was found to have potential antibacterial and mosquito larvicidal activity.

Keywords: Lactobacillus plantarum BCH-1, Bis-(2-ethylhexyl) phthalate, FT-IR, GC-MS, ESI-MS/MS, Antibacterial activity, Mosquito larvicidal activity

O-AIP13

Chitosan nanoparticles coated with curcumin as seed priming agents induce stress tolerance in wheat (Triticum aestivum L.) for sustainable growth

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Abstract

The germination, growth and development of wheat have greatly been affected by the ecotoxicological conditions and environmental stresses over the last few decades. The abiotic stresses induce negative impacts on metabolic processes, biochemical and physiological attributes. Consequently, the disturbed cellular pathways and disrupted metabolic functions inhibit plant growth and limit crop productivity. Over the last few years, chitosan nanoparticles (CNPs) have shown promising applications in agriculture. Seed priming significantly increases the peroxidase, protease, non-reducing sugars, CMS and relative water content in seedlings under normal and stress conditions. Considering the plant growth-promoting, immunomodulator and non-hazardous nature of chitosan and antioxidant potential of curcumin we prepared CNPs coated with curcumin as ecofriendly priming agents for wheat seeds. The effects of aforesaid priming agents will be discussed on biochemical attributes under normal and stress conditions. The priming effects on hydrolytic enzymes, important biomolecules, enzymatic and non-enzymatic anti-oxidants will be discussed on primed, hydro-primed and non-primed control seeds. Further, the stress emulating-role of aforesaid eco-friendly priming agents will be discussed on biochemical attributes of wheat seedlings originated from primed, non-primed and controlled seeds under normal and stress conditions.

Keywords: Seed programming, Seed pre-conditioning, MDA, nano-priming, sustainable

O--AIP14

Biochemical potential of Eucalyptus camaldulensis essential oils extracted by traditional and superheated steam extraction

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Abstract

Eucalyptus camaldulensis essential oil plays an important role in natural medicine due to its biological properties. The main objective of this research is to study the variation in yield, chemical constituents, antioxidant and antibacterial activities of Eucalyptus camaldulensis leaves essential oil extracted by hydro, steam, and superheated steam extraction. The experimental results showed that superheated steam extraction gave an optimum essential oil yield followed by steam and hydro distillation, respectively, with shorter extraction time. The GC-MS results showed that 1,8 cineole was the major constituent of essential oils followed by γ-elemene, piperitone, β-cymene, α-thujene, pinanediol and terpinen-4-ol. The components such as α-thujene and β-cymene, terpinen-4-ol and piperitone varied with extraction techniques. The essential oil extracted by superheated steam extraction showed highest antioxidant activity assessed by different extraction methods. Antibacterial activity of essential oils was determined by disk diffusion and resazurin microtiter plate assays. It was observed that hydro distilled essential oil showed the highest antibacterial activity against food borne disease causing bacteria. In conclusion, superheated steam extraction is an effective technique than conventional hydro and steam distillation in terms of essential oil yield and antioxidant activity.

O--AIP15

Chitosan nanoparticles coated with Moringa Oleifera extract as nano priming agent for physiological and biochemical alterations in wheat seeds

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Abstract

Wheat is an important staple food of Pakistan and its productivity is often encumbered by biotic and abiotic stresses including salinity. Chitosan is a natural biopolymer, biocompatible and non-toxic showing promising applications as a delivery agent for sustainable plant growth and crop productivity. The Moringa oleifera (MO) exhibits a broad range of bioactivities including high antioxidant potential. In this study, the chitosan nanoparticles (CNPs) were synthesized through ion gelation method and subsequently coated with extract of MO leaves. The prepared CNPs@MO were characterized using scanning electron microscopy, Fourier transforms infrared spectroscopy and X-ray diffraction analysis. The prepared nanocomposite was used as a wheat seed priming agent (0.02% and 0.04%). The primed, hydroprimed and non-primed control seeds were used for comparative physiological and biochemical analyses. The CNPs@MO caused a significant increase in enzymatic and non-enzymatic antioxidants to enable the germinating seeds to tolerate stresses. The nanopriming also induced a significant reduction in MDA contents along with an increase in other important biomolecules including proteins, sugars and osmolytes etc. The CNPs@MO-mediated physio-biochemical alterations in primed seeds invoked resistance to stresses in wheat seeds, a positive outcome for climate-smart agriculture.

Keywords: Nanopriming, sustainable agriculture, wheat, nanocarriers

O--AIP16

Increased Cl^-/SO_4^{2-} dialysis selectivity through polyelectrolyte multilayers coated aliphatic polyamide anion-exchange membranes

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Abstract

Highly selective monovalent to divalent anion-exchange membranes (AEMs) can find potential applications in areas such as separation and purification of salt mixtures. In this study, AEMs have been coated with poly(4-styrenesulfonate) (PSS)/protonated poly(allylamine) (PAH) multilayers to appreciably enhance the Cl^-/SO_4^{2-} transport selectivities in dialysis experiments. It was found that the increase in the monovalent to divalent anions selectivity is highly dependent on the source phase salt concentrations. The Cl^-/SO_4^{2-} selectivity through coated AEMs improved from 1.7 to 5.3 in diffusion dialysis when the source phase contained 0.01 M concentration with respect to each NaCl and Na_2SO_4 while the receiving phase contained 0.01 M Na_2CO_3. When the source phase concentration increased from 0.01 M to 0.1 M with respect to each NaCl and Na_2SO_4, the Cl/SO_4^{2-} selectivity increased to 140 in diffusion dialysis experiments. Even through unmodified AEMs, the selectivity increased to 13 with 0.1 M concentration of each salt in the source phase. Besides, AEMs modified only on the receiving side demonstrate much higher selectivities than those coated only on the source phase side. However, higher slectivities resulted in lower fluxes of ions. Partioning experiments show that high Cl^-/SO_4^{2-} selectivities at higher source phase concentrations partially stem from increased Cl^- partitioning. Moreover, modeling suggests that electromigration at higher source phase concentrations disproportionately decreases SO_4^{2-} flux in the AEM to yield enhanced Cl - /SO 4 2- Cl^-/SO_4^{2-} selectivities.

Keywords: anion-exchange membranes, dialysis, selectivity, polyelectrolytes, multilayers

O-AIP17

Assessment of different extraction parameters on phytochemical constituent's profile and antioxidant Potential of Dried Phlomis stwarrttii stem extract.

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Abstract

Sample preparation procedure before detection step is of great important for successful realization of analytical methods. Response surface methodology (RSM) based on three factors and three level Box Behnken design including 17 experimental design was used for optimizing the mechanical shaking extraction (MSE) conditions in methanol, such as solute to solvent concentration (10:100 mL, 10:150 mL, 10:200 mL), extraction time (2 h, 6 h, 8 h) and speed (100 rpm, 150 rpm, 200 rpm) for recovery of total yield, total phenolic contents (TPC) and total flavonoid contents (TFC) form flowers of Phlomis stewartii plant. Yield, TPC and TFC were studied by using second order polynomial equation. The optimum MSE condition was as follow: solvent concentration (200mL), time (8 h) and speed (150 rpm). Under these conditions, the run 4 showed significant results, which was comparable to predicted results. The lowest results for response were observed on following condition: solvent concentration was (100 mL), extraction time (2 h) and speed (100 rpm) shown by run 05. The run obtained at optimum MSE conditions were compared with those obtained less significant results; however, extraction time and solute to solvent concentration led to extract with highest yield, TPC and TFC. The results provide important guidance for quality evaluation and industrial application of Phlomis stewartii flower.

O-AIP18

Phytochemical Analysis of Different Extracts of Moringa Oleifera Seeds and Leaves

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Abstract

Medicinal plants serve as remedy against oxidative damage due to their activities against oxidative stress caused by free radicals, one of them is Moringa oleifera. This work was aimed to study the phytochemicals of Moringa oleifera seeds and leaves and their activity against oxidative stress. In this regard, the antioxidant activity of different extracts i.e., Methanol and n- Hexane extracts of Moringa oleifera seeds and leaves was studied. The DPPH radical scavenging assay along with Total Phenolic Content, and Total Flavonoids Content was performed in order to evaluate their antioxidant activity. The results revealed high potential to scavenge free radical with IC50 value as low as 40 µg/ml for Methanol extract of Moringa oleifera seeds and as low as 50 µg/ml for Methanol extract of Moringa oleifera leaves. While the remaining n-Hexane extract showed low scavenging activity. Moreover, the Total Phenolic Content and Total Flavonoids Content of Methanol extract of Moringa oleifera leaves exhibited higher content values than those for seeds and n-Hexane extracts. This study suggests that Phenolics and Flavoinoids are major phytochemicals responsible for significant antioxidant activity in Moringa oleifera seeds. Therefore, the role of Moringa oleifera as medicinal plant validates its use as antioxidant to cure oxidative stress related diseases.

O-AIP19

Efficacy of soil and foliar applications of chemically synthesized ZnO Nano fertilizer on morphological and nutritional quality of Zea mays crop: A comparison.

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Abstract

The primary goal of using Nano-fertilizers in agriculture is to reduce mineral fertilizer losses while increasing yields to promote agricultural output. In this context, the present study was conducted at Post agriculture research station (PARS) UAF, in the growing season of maize plant to investigate the efficacy of chemically synthesized Nano fertilizer of Zinc on the biochemical, morphological, physiological, nutritious quality and yield related parameters of maize. Despite the fact that ZnO is commonly researched on plats in many types of soils, the soil contains numerous nutrients, including some of the toxic components that might influence ZnO studies. As a result, the current investigation was conducted in double washed sand to remove all sand nutrients and components. The Zinc nanoparticles were synthesized chemically and characterized to investigate the size, surface morphology, dimensional structure and crystalline composition using SEM, XRD, FT-IR, and UV-Visible spectroscopy. The Nano-fertilizers were applied to plants using two techniques, through soil application and foliar application. For soil application, a maximum average increase of 61.1% in plant growth, 51.8% in photosynthetic pigments and 49.25% in anti-oxidant contents was observed as compared to control plant. For foliar application, an average increase of 59.28% in plant growth, 48.19% in photosynthetic pigments and 52.91% in anti-oxidant contents was observed as compared to control. The results suggests that, the ZnONPs have the potential to be employed as a Nano fertilizer for crops cultivated in Zn-deficient soils to boost agricultural output, food quality, and alleviate worldwide hunger.

Parallel Session III: Material Sciences

O-MS01

Effective photocatalytic degradation of Methylene Blue dye in waste water system using Manganese Ferrite Magnetic Nanoparticles

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Abstract

Manganese ferrite ($MnFe_2O_4$) was prepared via hydrothermal route and characterized by advanced techniques. The photocatalytic activity (PCA) was evaluated by degrading methylene blue (MB) dye under UV irradiation. The effect

of process variables such as catalyst dose, UV exposure time and pH was studied for maximum degradation of dye at optimum conditions. The MnFe2O4 showed face centered cubic structure and average particle size of 23.98 nm. The lattice constant, lattice strain, ionic radii (r A & r B), bonding angles and hoping lengths of $MnFe_2O_4$ were recorded to be 0.8467 nm, 0.08, 1.66, 0.766, 1.833 and 2.116 Å, respectively. The $MnFe_2O_4$ showed promising PCA and at optimum conditions of process variable, up to 99% MB dye degradation was achieved. The PCA was found dependent to catalyst dose, UV exposure time and pH. Results revealed that the hydrothermal rout is feasible route for the preparation of $MnFe_2O_4$ferrite in nano size and the PCA revealed the potential application of $MnFe_2O_4$ ferrite to degrade dye in textile wastewater.

O-MS02

Green synthesis of stable and monodisperse CuO nanoparticles using punica granatum extract as a reducing agent

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Abstract

In present study synthesis of Copper Oxide (CuO) nanoparticles was carried out in aqueous media by using peals extract of Punica granatum as reducing agent as well as capping agent. The optical, structural and catalytic properties of formed CuO nanoparticles were investigated. The reaction conditions including concentration of salt, pH of reaction medium, temperature of reaction system and time of heating of reaction medium were systematically optimized in order to get the best particle size and yield of nanoparticles. The optical and structural properties of CuO nanoparticles were investigated by employing various characterization techniques including UV/Visible spectroscopy, Fourier transform infrared spectroscopy and X-ray diffraction. Here, nickel nanoparticles were prepared from aqueous solution of nickel nitrate using aqueous extract of Punica grantum. The best yield of nanoparticles was obtained in plant mediated fabrication at pH 12 using 1M salt, temperature and heating time of 80C 0 and 60 minutes, respectively. The catalytic properties of plant were studied by conducting their photo-catalysis on methylene blue dye and 4-Nitrophenol.

O-MS03

Highly Efficient ZnO Nanorods as an Adsorbent for Cr (VI) Removal from Aqueous Solution

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Abstract

Zinc oxide (ZnO) nanorods were fabricated through hydrothermal route and employed for the adsorption of Cr (VI) ions from aqueous medium. Zinc nitrate hexahydrate ($Zn(NO_3)_2.6H_2O$) was used as a zinc precursor and Triton-x 100 was used as a capping agent. As synthesized ZnO nanorods were characterized by UV-visible spectroscopy (UV), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and energy dispersive X-Ray spectroscopy (EDX) techniques. The adsorption affecting parameters were investigated for maximum adsorption of Cr (VI) onto ZnO nanorods. The adsorption kinetics, isotherms, and thermodynamics were applied for adsorption mechanism evaluation. Maximum adsorption of Cr(VI) ions (250 mg/g) was achieved using 0.055 g/L ZnO dose at pH 2.0 for the contact time of 30 min. Pseudo-second-order kinetic model and Langmuir isotherm explained well the Cr (VI) adsorption onto ZnO nanorods. The Cr (VI) adsorption onto ZnO was spontaneous and endothermic in nature. In view of promising adsorption efficiency, ZnO nanorods could possibly be used for Cr (VI) ions removal from wastewater and also extendable for the adsorption of other heavy metals ions.

Key words: ZnO, nanorods, waste water treatment, adsorption, Cr (VI) removal, hydrothermal method,

O-MS04

Photocatalytic degradation of Metribuzin by Lab prepared mixed Oxide of Ti and Zn in aqueous solution

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Abstract

The present study was focused on preparation of mixed oxides of Zn and Ti by Sol gel process and characterizations of prepared TiO 2 /ZnO was performed using Fourier-transform Spectroscopy (FTIR), Scanning electron microscopy (SEM), and Energy Dispersive X-ray (EDX). The prepared TiO 2 /ZnO was utilized for degradation of metribuzin under influence of various operational parameters such as time of reaction, speed of agitation, dose of catalyst, initial concentration of metribuzin, pH of solution and· temperature. The results showed that degradation of metribuzin was depended on solution pH and maximum degradation was achieved at pH 6. The degradation study revealed that % degradation of metribuzin increased with progress of catalyst dose as well as temperature. The degradation studies were fitted into Arrhenius equation to calculate the activation energy and it was found to be 12.81 KJ/mol. Kinetics of the degradation of metribuzin was also studied.

O-MS05

Plant-mediated biosynthesis of zinc oxide nanoparticles for remediation of acid blue a dye

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Abstract

Nanotechnology is gaining popularity due to its multi applications in various applied fields like textile industry. The green synthesis of metal or metal oxide nanoparticles is an eco-friendly, stable, simple, rapid and cost-effective approach. In the current study, fruit peels extract of Punica granatum (Pomegranate) were utilized for the synthesis of zinc oxide nanoparticles (ZnO-NPs). The synthesized zinc oxide nanoparticles were characterized by different spectro-analytical techniques like SEM, XRD, FTIR etc. The particle size of ZnO nanoparticles was found to be 39-40 nm as shown by FESEM. Optimized conditions for the preparation of zinc oxide nanoparticles were found to be temperature 80 °C, pH 9, reactant ratio 1:5 and 80 minutes contact time. The ZnO nanoparticles were employed for the remediation of Acid Blue A dye following the optimization of experimental parameters like dye concentration (Acid Blue A), ZnO nanoparticles concentration, pH, dose of H_2O_2 and temperature. The Acid Blue A dye was 87% decolorized at 0.04 % dye concentration, 3 mg ZnO nanoparticles concentration, pH 6, 0.4 M H2O2 at 40 °C. Dye treated sample was subjected to chemical oxygen demand (COD) and total organic carbon (TOC) measurements. The COD and TOC values were found to be 90 % and 89.34 %, respectively. It can be concluded that synthesized ZnO nanoparticles successively degraded our targeted dye. These synthesized ZnO nanoparticles could be applied for the detoxification of other toxic dyes as well.

Keywords: Green synthesis of zinc oxide nanoparticles, SEM & XRD, detoxification of Acid Blue A dye, COD & TOC

O-MS06

Antioxidant, antidiabetic, antimicrobial, antihemolytic activities of gymnema sylvestre leaves extracts and chemical characterization – a nanotechnology approach

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Abstract

Plants have also been offered as conventional medicine and modern drugs to fulfill the health care needs of mankind. The current study was undertaken to assess antioxidant, antidiabetic, antimicrobial, and antihemolytic activities of Gymnema sylvestre leaves ethanolic extract (GSE) and nanosuspension (GSN). Antioxidant potential was checked by its total phenolic content (TPC), total flavonoid content (TFC), and 2, 2-diphenyl-1-picrylhydrazyl (DPPH) quantities in the Gymnema sylvestre. The antidiabetic potential was assessed by glycation and alpha-amylase

inhibition assays. Cytotoxicity was checked by a hemolytic assay. Structural characterization of Gymnema sylvestre was done to investigate bioactive compounds, using High-performance liquid chromatography and Fourier transform infrared spectroscopy techniques. According to the results obtained, 69.6 mg gallic acid equivalent / 100 g dry weight TPC in GSE and 11.84 mg gallic acid equivalent / 100 g dry weight TPC in GSN were measured. In TFC assay, 108.6 mg catechin equivalent / 100 g dry weight TFC and 130.53 mg catechin equivalent/100 g dry weight TFC were observed in GSE and GSN respectively. DPPH inhibitory potential of GSE and GSN was found to be 35.22% and 22.25 % respectively. Regarding antimicrobial potential, 62.08% and 69.12% inhibition of *E. coli*. Biofilm by GSE and GSN respectively was studied. Whereas, 80.67% and 40.33% growth inhibitory effects in the case of S. aureus were exhibited by GSE and GSN respectively. Biofilm inhibition of extract and nanosuspension was 62.08% and 69.12% against *E. coli* and *S. aureus* was 80.67% and 40.33% respectively. The antiglycation activity of GSE and GSN was 41.4% and 35.8% respectively and alpha-amylase inhibition by GSE and GSN was 19.5% and 5% respectively. Cytotoxicity capacity as determined by hemolytic assay was found to be 51.86% hemolysis for GSE and 33.63% hemolysis for GSN. The HPLC analysis indicated the presence of phenolic acids such as chlorogenic acid and gallic acid. FTIR spectrum revealed the presence of alkanes, aldehydes, sulfoxides and alcohols compounds. It is concluded that GSN is better in terms of some activities as compared to GSE. Further studies are warranted to explore proper medicinal attributes of Gymnema sylvestre

Keywords: Gymnema sylvestre, nanosuspension, antioxidant, antidiabetic, biofilm

O-MS07

Preparation of silica aerogel/glass fiber composites and role of supercritical CO_2 drying

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Abstract

Silica aerogel is a kind of amorphous mesoporous material with high specific surface area, low density, and high porosity, and is the best thermal insulation material to date. It has broad applications, such as in the thermal insulation material, chromatographic separation, and drug delivery system. However, the mechanical properties of the silica aerogel are poor. In our study, a new strategy was proposed to improve the mechanical properties of the composite without deteriorating its thermal insulation property. Given the problems of existing big void space in the composite of silica aerogel/glass fiber and the weak combination between them, and long drying period, the composite was prepared by using an acid-base catalyzed sol-gel and supercritical CO_2 drying method, and characterized and analyzed by SEM, TEM, BET, FTIR, constant thermal analyzer, mechanical compressing tester, etc. The effects of adding silica gel and gas-phase silica on the properties of the composites were studied. The effects silica gel/fumed silica and the co-precursors followed by supercritical CO_2 drying on the properties of the silica aerogel/glass fiber composite were investigated. Results showed that the thermal conductivity of the composites were not compromised. SEM images showed that the added silica gel/fumed silica filled the void spaces between the glass fiber and silica aerogel, acted as a bridge between them through the Si-O-Si network. The research results provide a new method for the preparation of excellent thermal insulation materials. **Keywords:** silica aerogel; glass fiber; silica gel; fumed silica; supercritical carbon dioxide.

O-MS08

Creating water-repellent effects on pine wood by TiO_2 incorporated fluorocarbon impregnations

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Abstract

Yellow pine wood was successfully treated with the titania incorporated fluorocarbon mixtures. In practice, wood samples were vacuum impregnated by these mixtures and subsequently were cured by using suitable in-house

developed protocols to optimize the properties of the treated wood. The main objective of this work is to tailor the water-related properties and impart hydrophobic features. Energy dispersive X-ray spectroscopy (EDS), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and water contact angle measurements (WCA) were employed to characterize the hydrophobicity of treated wood specimens. EDS, XRD, and FTIR proved that titania incorporated fluorocarbon blocks the OH component of wood surface through the combination of hydrogen groups during the impregnation. As a consequence of the treatment, wood gained weight (up to 3 %) and compacted its cell walls (up to 6%) due to the incorporation of the materials into cell lumen and cell walls. Treated wood exhibited better surface hydrophobation and took up considerably less water and moisture in comparison to untreated controls in water and moisture sorption tests. EMC and ASE values for treated samples were also very low (up to 66%) concerning untreated wood and were reduced by increasing titania content indicating that treated wood is more dimensionally stable and better bio-durable than untreated wood. The highest WCA reached 171º along with lowest concentration having contact angle 151º. It manifested that treated wood possessed a superhydrophobic surface. Since titania incorporated fluorocarbon is a low-cost promising approach to chemically modified wood with improved water and bio-resistant properties and has a huge potential to be commercialized in near future.

O-MS09

Photocatalytic performance of doped and undoped Strontium hexaferrite nanomaterials and their structural, morphological and dielectric properties

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Abstract

In current research efforts the Sr1-xCoxFe12-yCryO19 nanoparticles were synthesized via micro-emulsion route. The Effect of doping of Cobalt and Chromium ions on dielectric, morphological, structural, photocatalytic and optical properties of Sr1-xCoxFe12-yCryO19 was determined. The fabricated nanomaterials were characterized using X-ray diffraction (XRD), Scanning electron microscopy Raman spectroscopy, UV–Vis spectroscopy, Fourier transform infrared (FTIR). The XRD analysis confirmed formation of hexagonal M-type ferrites with average grain size of about 38 nm. Dielectric measurement revealed that the highly substituted nanomaterials have high dielectric constant and low current leakage versus SrFe12O19. The band gap energy decreased by the addition of sub band gaps and reduction of particle size. The photocatalytic activity (PCA) of Sr1-xCoxFe12-yCryO19 was evaluated by degrading the Rhodamine B (RhB) dye under solar light irradiation. The Sr1-xCoxFe12-yCryO19 degraded up to 87.6% of dye in 45 min of solar light irradiation with rate constant of 0.03834 min^{-1}. Results revealed that the high electrical conductivity and tuned band gap of these fabricated materials make them feasible for the efficient utilization in photovoltaic cells, SOFCs and as an encouraging photocatalyst for waste-water treatments.

O-MS10

Synthesis, Characterization and therapeutic potential of zinc oxide nanoparticles from Catharanthus roseus leaf extracts

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Abstract

Nanoparticles synthesis using plants with biomedical applications is a safe, cost-effective, biocompatible and eco-friendly approach. Anticancer activity of zinc oxide nanoparticle (ZnONPs) varies with plant to plant and biosynthesis of ZnONPs using different plants and plant source (leaves, flower, fruit etc.) with morphology and size show different efficacy towards cytotoxicity of cancer cells. In this study leaves of Ficus religiosa and Catharanthus roseus are the native plants used for the synthesis of zinc oxide nanoparticle (ZnONPs) for their anticancer activity. This study was aimed to investigate the anti-cancer activity of green synthesized ZnNps against MCF-7 cancer cell lines in the direction of development of more potent anticancer drugs. Zinc nanoparticles were synthesized by a green

route using an aqueous and methanolic extracts of both plants and were characterized by FTIR, XRD, and SEM. The cytotoxic effect of ZnNP of Ficus religiosa and Catharanthus roseus against MCF-7 was confirmed with MTT assays. These palnt nanoparticle showed a good activity against cancer lines. Perhaps this will be the first report on anti-cancer property of ZnONPs on MCF-7 in the field of cancer. This work will prove the efficacy/potency of ZnONP in the field of cancer and thus in further studies can be rationalized as potent anticancer agents due the presence of active constituents found in these plants.

O-MS11

Thermal conductivity of single-walled carbon nanotubes using molecular dynamics simulations

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Abstract

Carbon nanotubes (CNTs) are considered to be best candidate for thermal conduction and management in nano scale devices. Role of size, defects, grain boundaries become more prominent as we go down the length scale. Influence of chirality and length on thermal conductivity of single walled carbon nanotubes (SWCNTs) at different temp ranges is discussed to understand and develop efficient nanotube systems with desired thermal characteristics. Length of SWCNT is varied from 100A to 900A for both armchair and chiral configuration. Equilibrium Molecular Dynamics (EMD) is implemented by using LAMMPS with REBO potential. For shorter lengths, impact of chirality is more obvious. Decreasing pattern is observed with rise in temperature because of increase in thermal resistance. The results of present work provide deep understanding of thermal conductivity dependence on temp and length.

O-MS12

Exploration and tuning of intrinsic mobility and optoelectronic properties of organic semiconductor materials

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Abstract

The organic π-conjugated materials have considerable interest in semiconductor devices. The organic semiconductor materials (OSMs) are efficient to be used in photovoltaics, organic field effect transistors, laser technology, electroluminescent and electronic devices. Numerous OSMs like polycyclic organic compounds are most important players in the field of electronics. We have explored the optoelectronic properties and intrinsic mobility of various compounds by advanced computational approaches then compared the data with experimental and/or computed evidence. Additionally, we have designed various new compounds by multiple strategies with the aim to tune their properties of interests. Effect of various functionals and basis sets was systematically studied and compared. The effect of donor (D), acceptor (A), π-bridge was investigated on the charge transport and optoelectronic properties at molecular and bulk scales e.g., frontier molecular orbitals (FMO), absorption, fluorescence, transfer integrals, electron affinity (EA), ionization energy (IE), reorganization energy, density of states, conductivity, dielectric functions, refractive indices and extinction coefficient. The hole and/or electron transfer nature of the OSMs was evaluated by shedding light on the transfer integrals, reorganization energies and intrinsic mobility. Some multifunctional materials were proposed with enhanced properties than parent compounds with anticipation that such compounds would be suitable to be used in semiconductor devices.

O-MS13

Synthesis and Characterization of Lanthanum Substituted Manganese Spinel Ferrite ($MnLa_xFe_{2-x}O_4$) Nanoparticles

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Abstract

A series of lanthanum substituted manganese spinel ferrites ($MnLa_xFe_{2-x}O_4$) have been synthesized by sol-gel auto combustion route and prepared five samples by varying lanthanum concentration from x = 0.00 to x = 0.20. The annealing was done at 600 ^{0}C for three hours for all samples to obtain crystalline structure. Different characterization techniques have been adopted to explore the nature and properties of the prepared compound. X-ray Diffraction Analysis (XRD) aided in investigating the variations in different structural properties due to the substitution of Lanthanum ion, such as lattice constant, crystallite size, x-ray density, bulk density, dislocation density, micro strain, stacking fault and surface area. The presence of FCC phase in the XRD spectrum confirmed the spinel nature of the particles, which have been further confirmed by FTIR analysis. The crystallite size has been estimated by different methods including Scherrer method, Williamson Hall method, Size strain method and modified Scherrer method, all comparable to each other. The average crystallite size ranges from 9.7 to 11.6 nm. The synthesized particles be potentially applied in high storage devices, supercapacitors, batteries etc. Scanning Electron Microscopy helped in studying the surface morphology of the prepared ferrite material. By using LCR meter, dielectric properties of the prepared particles like complex impedance, dielectric constant, electric modulus, tangent loss and AC conductivity have been analyzed by varying frequency from 1 MHz to 3 GHz. The dielectric parameters have been studied by Maxwell Wagner Model and Koop's phenomenological theory. The obtained results of complex impedance, electric modulus and AC conductivity revealed that our fabricated compound has excellent insulating properties at low frequency domain and can have good applications in microwaves devices.

O-MS14

Photovoltaic Properties of ZnO Films Co-Doped with Mn and La to Enhance Solar Cell Efficiency

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Abstract

In the present investigation, ZnO films co-doped with Mn and La were synthesized by the sol–gel technique. XRD analysis revealed that ZnO had a hexagonal structure. Mixed hexagonal and cubic phases appeared in ZnO containing Mn (1%) and La (1.5%). The grain size, d-spacing, unit cell, lattice parameters, atomic packing fraction, volume, strain, crystallinity, and bond length of co-doped ZnO films were determined as a function of doped ion contents. Through UV analysis, it was found that pristine ZnO had Eg = 3.5 eV, and it decreased when increasing the doping concentration, reaching the minimum value for the sample with 1% Mn and 1% La. The optical parameters of the films, such as absorption, transmittance, dielectric constants, and refractive index, were also analyzed. DSSCs were fabricated using the prepared ZnO films. For pure ZnO film, the values were: efficiency = 0.69%, current density = 2.5 mAcm-2, and open-circuit voltage = 0.56 V. When ZnO was co-doped with Mn and La, the efficiency increased significantly. DSSCs with a ZnO photoanode co-doped with 1% Mn and 1% La exhibited maximum values of Jsc = 4.28 $mAcm^{-2}$, Voc = 0.6 V, and efficiency = 1.89%, which is 174% better than pristine ZnO-based DSSCs. This material is good for the electrode of perovskite solar cells.

O-MS15

Structural, dielectric, impedance and electric modulus properties of Ni0.5Mn0.5Fe2O4/La0.2Bi0.8FeO4 nanocomposites

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Abstract

In this paper, Ni0.5Mn0.5Fe2O4/La0.2Bi0.8FeO4 (NMFO/LBFO) nanocomposites were prepared by sole gel auto combustion method while bearing concentration is 0.1, 0.2, 0.3, 0.4 and 0.5. All these samples were annealed at 600 ºC for 3 hours in a muffle furnace to achieve crystalline nature of the prepared ferrites. The crystalline structure was studied through the X-ray diffraction (XRD) Technique. Vibrating sample magnetometry (VSM) was use to determine the magnetic properties of the synthesized composites and it was found that with the enhancement of NiMnFe2O4, magnetic characteristics were significantly improved. The surface morphology was performed by the scanning electron microscopy (SEM). The presence of functional groups of the prepared nanoparticles was investigated by Fourier transform infrared spectroscopy (FTIR). The electrical properties were determined using the impedance analyzer with applied frequency range of 1 MHz to 3 GHz. It was found that both the real and imaginary parts of the dielectric constant decreased with increasing applied frequency. Furthermore, there are some relaxation peaks observed at high frequency. The significant variations were found when concentration varied. In conclusion, the obtained magnetic and dielectric values suggested that the prepared nanocomposites would be possible for energy storage applications.

O-MS16

Study of Neodymium ion (Nd^{+3}) doped Manganese-Cobalt (Mn-Co) mixed spinel ferrite nanoparticles for Energy Storage Applications

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Abstract

The electrical and magnetic properties of cubic spinel ferrites are currently in focus due to their diverse applications, like magnetic resonance, transformer cores, targeted drug delivery, magnetic storage devices and microwave devices. In this work, Nd doped Manganese-Cobalt spinel ferrite ($Mn_{0.7}Co_{0.3}Nd_xFe_{2-x}O_4$) were prepared in powder form via Sol-Gel auto-combustion technique with concentration of step size = 0.05 and (x = 0.0-0.2). The prepared samples were grinded and annealed at 600ºC for 4 hours. X-rays Diffractrometry (XRD), Fourier Transform Infrared Spectroscopy (FTIR), impedance spectroscopy and Vibrating Sample Magnetometer (VSM) were used for the structural, electrical, and magnetic properties analysis. XRD pattern confirms the formation of pure single phase FCC structure of Nd^{+3} doped Mn-Co ferrites. The crystallite size decreases from 19 nm (x = 0.00) to 14 nm (x = 0.10). The lattice parameter, lattice strain and stacking fault were also determined. FTIR analysis showed two characteristic absorption bands of ferrites which confirm the vibration of M-O(Metal-Oxygen) bond stretching, first band lies around 540cm^{-1} correspond to tetrahedral site, and second band was observed in the range of 410 cm^{-1} correspond to octahedral site. Hysteresis loop obtained from VSM data confirmed the soft ferromagnetic behavior of Mn-Co spinel ferrites. Further, it is found that Coercive Field and remnant magnetization is decreasing with the increase in Nd concentration. The saturation magnetization is increasing with the increase of Nd concentration. This study reveals

that optimal soft magnetic behavior is obtained with doping concentration of (x = 0.15). The study of dielectric properties of interest (complex dielectric constant, dielectric tangent loss, impedance, A.C. conductivity, and electric modulus) as a function of the Nd doping concentration was carried out in the frequency range from 1MHz to 3GHz using an impedance analyzer. On the basis of these investigations, it was found that dielectric constant remains stable upto 1.5 GHz and two relaxation peaks were found in high frequency region that are around 1.8 GHz and 2.4 GHz. Cole–Cole plots of electric modulus revealed evidence of contribution from grains and grain boundaries in the conduction mechanism. This study shows that doping of Nd in Mn-Co ferrites make it suitable candidate for soft magnetic applications. Further these ferrites are also suitable for microwave wave devices in the specified frequency range.

O-MS17

Synthesis and characterization of (x)Cu0.05Co0.95Fe2O4/(1-x)La0.15Bi0.85FeO3 Nanocomposites

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Abstract

Nano-materials and nanocomposites have a big share in technological advancement. Synthesis of nanocomposites are promising new opportunities in modern technical progress especially in microelectronics and high storage devices. Preparation of nanocomposites using Cu-doped Cobalt ferrite (CFO) and La-doped Bismuth ferrite (BFO) was done by sol-gel auto-combustion method for different concentrations (x = 0.1, 0.2, 0.3, 0.4 and 0.5). The all samples were annealed at 600 ^{o}C for crystal structure development. Formation of the composite was confirmed by XRD analysis. Plot of low frequency region of real part of impedance showed the active nature of grain boundaries. Real modulus M' response confirmed the electrode effect while real and imaginary dielectric plots show high response at different frequencies. Sharp peaks were obtained in real and imaginary dielectrics which are due to sudden dissipation of energy at a particular frequency. These results show high electrically active nature of the composite

O-MS18

Synthesis and characterization of (x)$Cu_{0.05}Co_{0.95}Fe_2O_4$/(1–x)$La_{0.15}Bi_{0.85}FeO_3$
Effect of Ce^{+3} doping on structural, magnetic, and electrical properties of Manganese-Zinc (Mn-Zn) mixed spinel ferrite nanoparticles

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Abstract

The electrical and magnetic properties of cubic spinel ferrites make them useful for a variety of applications, such as ferro-fluids, magnetic resonance imaging (MRI), data storage, and energy storage devices. The electrical conductivity of spinel ferrites is low as compared to other magnetic materials, which make them a suitable candidate for microwave applications. In this work, a series of Cerium (Ce) doped Manganese-Zinc (Mn-Zn) ferrites $Mn_{0.7}Zn_{0.3}Fe_{2-x}Ce_xO_4$ were synthesized using the Sol–gel auto-combustion method with doping concentrations (x = 0.0, 0.05, 0.1, 0.15, and 0.2). The prepared samples were annealed at 600^{o}C for 4 hours to improve crystalline property. Structural properties were determined with the help of X- ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The effect of Ce doping on magnetic and electrical properties of Mn-Zn ferrites were determined by using VSM and Impedance Spectroscopy respectively. XRD analysis confirms the existence of pure FCC spinel phase. No impurity peak was detected which suggest that adequate amount of Ce^{+3} cations in Mn-Zn ferrite can substitute the Fe^{+3} ions on octahedral sites. The lattice parameter, lattice strain and stacking fault were also determined. The lattice constant decreases with Ce^{+3} ions replacement. Crystallite size of as prepared samples were determined by Debye–Scherrer

formula. The crystallite size was found in the range of 14 to 18 nm. FTIR result shows two characteristics bands near about 540 cm^{-1} and 410 cm^{-1} which confirms the formation of tetrahedral and octahedral sites of spinel ferrite. Magnetic measurements were done by VSM which reveal that coercivity increases whereas, saturation magnetization, and remnant magnetization decreases with the doping of Ce ions. Tangent loss (tanδ), dielectric constant, and dielectric loss values are determined in the 1 MHz to 3 GHz frequency range, and explained by the Maxwell–Wagner model. A persistent behavior of dielectric loss and dielectric constant was found before the microwave frequency region. The dielectric constant versus frequency analysis indicate three relaxation peaks at 1GHz, 1.8 GHz and 2.5 GHz. Ac conductivity and impedance of as prepared samples is also determined in the 1 MHz to 3 GHz region, and is found to be impacted by grain and grain boundary resistive behavior at low and high frequencies. Cole–Cole plots of different samples, corresponding to different doping concentrations, are used to describe the conduction phenomena. The doping of Ce ions enhances the coercive behavior of Mn-Zn mixed ferrites

O-MS19

Improving the Structural, Optical and Photovoltaic Properties of Sb- and Bi- Co-Doped $MAPbBr_3$ Perovskite Solar Cell

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Abstract

The electrical and magnetic properties of cubic spinel ferrites make them useful for a variety of applications, such as ferro-fluids, magnetic resonance imaging (MRI), data storage, and energy storage devices. The electrical conductivity of spinel ferrites is low as compared to other magnetic materials, which make them a suitable candidate for microwave applications. In this work, a series of Cerium (Ce) doped Manganese-Zinc (Mn-Zn) ferrites $Mn_{0.7}Zn_{0.3}Fe_{2-x}Ce_xO_4$ were synthesized using the Sol–gel auto-combustion method with doping concentrations (x = 0.0, 0.05, 0.1, 0.15, and 0.2). The prepared samples were annealed at 600 ^oC for 4 hours to improve crystalline property. Structural properties were determined with the help of X- ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The effect of Ce doping on magnetic and electrical properties of Mn-Zn ferrites were determined by using VSM and Impedance Spectroscopy respectively. XRD analysis confirms the existence of pure FCC spinel phase. No impurity peak was detected which suggest that adequate amount of Ce^{+3} cations in Mn-Zn ferrite can substitute the Fe^{+3} ions on octahedral sites. The lattice parameter, lattice strain and stacking fault were also determined. The lattice constant decreases with Ce^{+3} ions replacement. Crystallite size of as prepared samples were determined by Debye–Scherrer formula. The crystallite size was found in the range of 14 to 18 nm. FTIR result shows two characteristics bands near about 540 cm^{-1} and 410 cm^{-1} which confirms the formation of tetrahedral and octahedral sites of spinel ferrite. Magnetic measurements were done by VSM which reveal that coercivity increases whereas, saturation magnetization, and remnant magnetization decreases with the doping of Ce ions. Tangent loss (tanδ), dielectric constant, and dielectric loss values are determined in the 1 MHz to 3 GHz frequency range, and explained by the Maxwell–Wagner model. A persistent behavior of dielectric loss and dielectric constant was found before the microwave frequency region. The dielectric constant versus frequency analysis indicates three relaxation peaks at 1GHz, 1.8 GHz and 2.5 GHz. Ac conductivity and impedance of as prepared samples is also determined in the 1 MHz to 3 GHz region, and is found to be impacted by grain and grain boundary resistive behavior at low and high frequencies. Cole–Cole plots of different samples, corresponding to different doping concentrations, are used to describe the conduction phenomena. The doping of Ce ions enhances the coercive behavior of Mn-Zn mixed ferrites

Parallel Sessions V: Theoretical and Applied Physics

O-TAP01

Recent R&D activities at Atomic and Laser Physics, NCP Islamabad

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Abstract

Our country has very limited resources for research work at the public sector universities. Therefore, our government decided to build the National Centre for Physics (NCP) in Islamabad to provide centralized experimental facilities to the research students from all over the country especially to the less privileged universities, where such facilities are not available. The well-trained graduates of these universities will provide the *trained manpower* to the R&D sectors of Pakistan. *The Human Resource can't be developed without having in-house experimental facilities at NCP***.** The atomic and laser physics department can be considered as a backbone in the field of Lasers and Applied research. Therefore, we are in the process of establishing the Atomic and Laser Physics Laboratory at NCP. The Pakistan Academy of Sciences provided financial support RS. 11.0M to initiate this laboratory. However, this amount was not adequate for expediting the idea of a well-established Atomic and Laser Physics Laboratory at NCP. Another project of Rs. 70M approved by PSDP for the upgradation of Atomic and Laser Physics Lab. at NCP. It is worth mentioning that these experimental facilities functioning at NCP will be available to the research scientists/scholars/students/faculty members from all over the country according to the rules and regulation. The students from any research organizations/ universities will benefit from this facility. This will facilitate the research activities and institutional capacity building as research scientist from R&D sectors and students from the public sector universities will be trained. In this talk; I will briefly introduce the recent R&D activities at our Lab and opportunities of your M. Phil/PhD Scholar and faculty members from all over the country.

O-TAP02

Assessment of soft tissue substitutes for megavoltage photon beams

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Abstract

Due to the elevation in modern technology together with medical physics, various methods for radiation therapy treatment for various clinical purposes are being applied these days. Also, the development in simulation has turn

out to be the most important technique as in order to minimize the dissimilarities between the calculated dose distribution, phased at treatment planning and those distributed to the patient. It includes EGSnrc based Monte Carlo codes. In the present work, three phantom materials including Mylar, Nylon and Polyethylene were assessed for soft tissue equivalence at two mega-voltage photon beams and field sizes. BEAMnrc and DOSXYZnrc were employed for LINAC head modelling and phantom dose calculations respectively. Photon beams of 6 MV and 10 MV energies were assessed for their interactions in all the mediums. Gamma index and PDDs were recorded for two field sizes i.e. 5×5 cm2 and 10×10 cm2. Nylon was found to be the best among all other mediums under consideration in this work

O-TAP03

Photocatalytic degradation of Methyl Green dye mediated by pure and Mn-doped Zinc Oxide nanoflakes under solar light irradiation

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Abstract

Herein we describe an effective route for the degradation of methyl green (MG) dye under visible light illumination by Pure and manganese (Mn)-doped zinc oxide (ZnO) photocatalysts (synthesized by the simple chemical precipitation method). The X-Ray Diffraction (XRD) structural analysis has confirmed that both photocatalysts exhibit the hexagonal wurtzite structure; without any additional phase formation in Mn-doped ZnO, in particular. The optical properties of the synthesized photocatalysts have been investigated using UV–vis absorption spectroscopy in the wavelength range of 300-800 nm. Through Tauc's plot, the slight increase from 3.3 to 3.4 eV in bandgap energy has been elucidated in the case of Mn-doped ZnO. The morphological study has also been performed using Field Emission Scanning Electron Microscope (FESEM), which indicates nanoflakes (NFs) based surface texture for both photocatalysts. During the photocatalytic activity study, within 60 min irradiation of natural sunlight, ~62.78% and ~66.44% photocatalytic degradation of MG aqueous solution has been achieved mediated by pure and Mn-doped (2 wt.%) ZnO photocatalyst, respectively. The rate of photocatalytic reaction (K) ~ 0.01477 min -1 and R 2 ~ 0.92164 has been achieved for pure ZnO, whereas slightly higher ~ 0.01617 min -1 and R 2 ~ 0.93494 has been observed for Mn-doped ZnO photocatalyst. The significantly improved photodegradation activity of Mn-doped ZnO may be ascribed to the relatively higher surface defects, improvement of e^-/h^+ pair charge separation and efficient generation of hydroxyl radicals mediated by Mn-doped ZnO photocatalyst.

Keywords: Chemical precipitation method; pure ZnO nanoflakes, Mn-doped ZnO; Photocatalytic activity; Methyl Green, Wastewater treatment.

O-TAP04

On dynamics of anisotropic compact stars in rainbow gravity Umber Sheikh

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Abstract

Compact objects are the final fate of collapse, an important phenomenon in stellar creation. This work is devoted to analyzing the evolution of compact stars from an anisotropic string fluid using the Karori- Barua metric. The Einstein field equations are modified in the regime of Rainbow Gravity. The dynamical variables of the string fluid including mass density, pressure, and string density are explored. These variables would be graphically

presented based on the radial distance and energy of the probing particle. Consequently, the energy conditions would be presented for the existence of a physical model.

O-TAP06

Estimation of ABC and GA Indices of Fullerenes

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Abstract

Fullerenes are the wonderful carbon allotropes used in different industries. The atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are two well-studied topological indices and are useful in determining the heat of formation of molecules. In this work, I shall calculate the ABC and GA indices of different fullerenes. Further, their linear relationship (regression relation) with the heat of formation will be determined. Moreover, the interrelationship of indices will be graphically presented and correlation will be interpreted.

O-TAP07

Synthesis, characterization, and antimicrobial application of $Mg_xZn_{1-x}Fe_2O_4$

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Abstract

In the present study, magnesium zinc nano ferrites were synthesized by using co-precipitation technique, after calcination and post-heating $MgCl_2$ utilized as a precursor. The chemical co-precipitation technique is very simple, appropriate, and helpful for the preparation of different types of nanoparticles due to its better results, regarding crystallite size and other properties. An aqueous solution of magnesium zinc ferrites was prepared by dissolving into deionized water and other solution sodium hydroxide (NaOH) was gradually mixed by applying constant stirring until the pH of the material reached up to 14. As a result of this mixing, precipitates were formed. These precipitates were washed repeatedly with deionized water and ethanol till pH reached to 7. These washed precipitates were passed through the process of drying and calcination. The post calcination process was also applied for the improvement in the purification and crystallinity of synthesized material. Characterization of the prepared material was accessed with the help of different techniques, including scanning electron microscopy (SEM) to the study of morphology, X-ray diffraction (XRD) to study the different structural parameters. Fourier transformation infrared radiation (FTIR) analyses were also used to confirm the presence of component materials. To test antibacterial activity, the synthesized nano materials were treated with Gram-positive, S. aureus, and Gram-negative K. pneumoniae bacteria. The inhibition activities of synthesized material were compared with the Gold standard (Ciprofloxacin).

O-TAP08

Assembly of CNTs coated stretchable fabric for the fabrication of wearable strain sensors

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Abstract

To detect the human motion, we need highly sensitive and stretchable strain sensors. Here, we report a highly stretchable, flexible and sensitive strain sensor fabricated using CNTs as a sensing material. The CNTs have been coated on a flexible textile fabric using a spray coating method. SEM is used to observe the embedded CNTs which behave as channel among different fibers. The sensitivity measurements suggested that the CNTs coated strain sensor offers flexibility, stretchability and good sensitivity with a high gauge factor. Such kind of sensors have high potential to detect human motion particularly where large deformation produces structural changes.

O-TAP09

Soft tissue and water substitutes for Megavoltage photon beams: An EGSnrc based evaluation

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Abstract

In this work, soft-tissue equivalence of water, polystyrene, PMMA and water equivalence of polystyrene, and PMMA has been assessed for multiple megavoltage photon beams and field sizes. EGSnrc based Monte Carlo (MC) codes, BEAMnrc and DOSXYZnrc are used for the linac head modeling and the phantom dose calculations, respectively. Percentage depth doses (PDDs) are scored for two field sizes and photon energies (6 MV and 10 MV) in water, polystyrene, PMMA, and soft tissue. The comparisons of PDDs show that soft tissue equivalence of various materials varies with the depth in the phantom, field size, and photon energy. Water and PMMA are found to be the closest soft-tissue and water substitutes, respectively. Soft-tissue and water equivalence of dosimetry materials need to be evaluated for a range of photon energies and field sizes before their application in complex radiation beams.

O-TAP10

The effect of laser irradiation on germination and seedling growth of Brinjal seed (*Solanum melongena*)

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Abstract

Laser is an optical instrument that produced the high beam of monochromatic light by the process of stimulated emission of radiation. Laser has many applications such as in industry, barcode scanners, and especially in agriculture to increase the seedling process, sprouting rate yield of different crops. Keeping in this view that the present study will be designed on the used of laser in agriculture. For this purpose, the semiconductor diode will be used to irradiate the brinjal seed before sowing. In this process Diode laser of 1mW power of wavelength 630 nm was apply to irradiate the brinjal seeds for different energy and time. For this purpose, fine, and fresh seeds of known variety chosen. The laser beam directly falls on the seed of brinjal for different time duration. Each treatment will be comprised on three replications, including control. Different physical parameter shoots and root length, germination rate dry and fresh weight etc studing during whole time period. Different biochemical parameters such as enzyme activities, mineral content, proteins etc will also be examine. In order to see the difference between treated and non-treated seeds the whole data will be analysis statistically.

O-TAP11

Molecular dynamics simulations of dynamical analysis in weakly coupled dusty plasmas

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Abstract

Dynamical structure factor (DSF) of three dimensional (3D) weekly coupled plasmas has been investigated by using equilibrium molecular dynamics simulation (EMD). The influence of variable wave number on the dynamical structure factor has been tested by using different values of plasma parameters coulomb coupling strength (Γ) and Debye screening strength (κ). Simulation work is done for testing influence of different wave vector on plasma density by using different states. The result of simulation technique for varying values of plasma parameters and number of particles shows the transitory behavior of frequency. The obtained result by using EMD is satisfactory as compared to earlier numerical and experimental results. At intermediate to higher values of

coulomb coupling parameter the oscillations of dynamical density S(k, ω) increases and with increasing number of particles dynamical density decreases. The result shows the less fluctuation at the higher ranges of Debye screening strength.

O-TAP12

Application of surface-enhanced Raman spectroscopy for pharmaceutical sciences

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Abstract

Surface-enhanced Raman spectroscopy is the most widely used technique in pharmaceutical sciences. It is a powerful method to detect different molecules on metal surfaces. Recognition of different small amounts of pharmaceuticals and different contaminants present in pharmaceutical samples is the main challenge in clinical diagnostics and protecting our environment. This work includes a low amount of pharmaceutical sample preparation methods. By using SERS micro-level samples of different pharmaceutics are used. After obtaining spectra from Raman spectroscopic instrument, data is processed through Matlab software containing different statistical tools for further accuracy. The great benefit of this type of approach is its high reliability and simplicity. Several related works have been done and it is a challenge to overcome further hurdles in pharmaceutical sciences.

O-TAP12

Application of surface-enhanced Raman spectroscopy for disease diagnosis

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Abstract

Different diseases are the major reason for the number of deaths globally. Primary diagnosis and treatments now have become productive routes for the control of increased death rates. There are huge challenges for detecting severe diseases with better sensitivity. In the modern years, surface-enhanced Raman spectroscopy (SERS) appeared as the most popular practice for the detection of different diseases like Cancer, Hepatitis, Tuberculosis, Diabetes, etc. SERS identifies diseases with great efficiency and potential for clinical detection. To collect different spectra, the required samples are examined by applying the SERS technique. After the collection of no. of spectra, different statistical tools are used like PLDA, PLSR, etc using computational software. In this field, very effective work has been done in the current 5 years and there are future challenges as well.

Keywords: Raman Spectroscopy; SERS; Disease Detection; spectroscopic analysis; Cancer; Hepatitis; Diabetes; tuberculosis; biomolecules; multivariate data analysis

O-TAP13

Theoretical investigations of TPA-DCPP based derivatives via structuralvmodification of donor fragment

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Abstract

So far, thermally activated delayed fluorescence (TADF) materials of red, blue, and green colors are often used in highly-proficient organic light-emitting diodes (OLEDs). However, because of the difficulties in molecular design, effective TADF materials with the color varying from red towards near-infrared (NIR) color are infrequently described. Herein, we are going to present a theoretical investigation of singlet-triplet energy gap (ΔE ST) and emission wavelength (λ em) of NIR-TADF materials via structural modification of the donor fragments on the parent molecule Triphenylamine dicyanopyrazino Phenanthrene (TPA-DCPP). The incorporation of different donor fragments like phenoxazine (PXZ), phenothiazine (PTZ), and carbazol (Cz) with various electron-donating strengths has shown a very small ΔE ST value of 0.06-0.09 eV and λ em in the near

infra-red region (660-680 nm.) We hope our theoretical investigation might offer hints for the production of highly-efficient TADF-OLEDs in the future.

POSTER PRESENTATIONS

P-01

Sub-chronic toxicity profile of methotrexate loaded chitosan and solid lipid nanoparticles in rodent model

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Abstract

Methotrexate (MTX), analogous to folic acid, is used in the treatment of rheumatoid arthritis. Chitosan is biocompatible and biodegradable biopolymer with biosafety profile. Lipid nanoparticles (NPs) have distinct characteristics which make them attractive carriers. MTX associated adverse drug reactions include neurotoxicity, hepatotoxicity, acute kidney injury and myelosuppression. These problems may be resolved by formulating MTX loaded chitosan and solid lipid NPs. This study aimed to prepare MTX loaded chitosan as well as solid lipid NPs and investigated their safety. The prepared NPs were characterized for zeta size and potential. The duration of the study was 42 days. Twenty albino rats were randomly divided in four groups. 1st group served as normal control while 2nd group was standard control with commercially available MTX. 3rd group was treated with MTX loaded chitosan NPs while 4th group was MTX loaded solid lipid nanoparticles. The particles size was found to be 200nm, 198.5nm while zeta potential was 30.4mV and -18.4mV for chitosan and solid lipid NPs respectively. The encapsulation efficiency was found to be 87.772% and 76.208%. The results of complete blood count (blood cells and erythrocyte indices) as well as liver (ALT, AST, ALP) and kidney function tests (creatinine and blood urea nitrogen) revealed that NPs may be considered safe. The oxidative stress parameters (SOD and CAT) in sera showed that NPs reduced the production of free radicals. The present study showed that methotrexate loaded chitosan and MTX loaded solid lipid NPs were less hepatotoxic and nephrotoxic than the pure drug.

P-02

Effect of environmental variables on the synthesis of Iron oxide nanoparticles synthesized from Plumeria obtusa aqueous extract: An optical study and characterization

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Abstract

Green synthesis of metals nanoparticles by means of aqueous plant extracts as reducing agents proves to be eco-friendly, economic and simple. In this study, synthesis of iron oxide nanoparticles (IONPs) was carried out using Plumeria obtusa leaves extract. The variation in concentration of iron salt, extract volume, temperature, pH and time of reaction were assessed to optimize size and shape of IONPs. The Ultraviolet/visible (UV/Vis) spectroscopy, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), X-ray diffraction (XRD) as well as energy dispersive X-rays (EDX) analysis were performed for characterization. The UV/Visible analysis confirmed the synthesis of IONPs with characteristic peak attained at 280 nm. Through optimization study, concentration of iron salt, extract volume, temperature, pH and time of reaction were analyzed as 1 mM, 20 mL, 50 oC, pH 6 and 24 hr respectively. FTIR analysis depicted the presence of alcoholic, alkanes and aldehydic groups in the Plumeria obtusa extract and their contribution in the synthesis of IONPs as clear shifting of peaks was observed. The spherical and rod shaped polydispersed, crystalline, cubic and metallic form of IONPs were visualized via SEM micrographs, XRD image and EDX profile.

Keywords: synthesis; nanoparticles; extracts; characterization; polydispersion

P-03

Developing Molecular Imprinted Magnetic Particles for Recognition of Cholic Acid

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Abstract

Cholic acid is an important human bile acid which is produced by liver from cholesterol metabolism. The concentration of bile acids is associated with proper functioning of liver therefore, its quantification is imperative in view of diagnosing hepatic diseases. In the current work, we developed molecular imprinted magnetic particles as affinity sorbent for recognition of cholic acid. Iron oxide nanoparticles are synthesized by co-precipitation method and used as supporting material that were integrated with acrylic based polymer system having cholic acid as template molecule. The structural characterization of as-prepared molecular imprinted magnetic particles is carried out by FTIR while the morphological features are studied by atomic force microscopic images. The magnetic particles demonstrated significant rebinding performance towards cholic acid comparing to control material.

P-04

Functionally modified C_{60} fullerenes as an efficient nonlinear optical material: A quantum chemical study

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Abstract

It is well-known that π-conjugation plays an important role to tune the nonlinear optical (NLO) response of donor-π-conjugated-acceptor compounds. In the present study, we systematically designed C_{60} derivatives (2 (fulleropyrrolidine) and 2a-2c (fulleropyrrolidine tetrathiafulvalene derivatives where 2a, 2b and 2c are with n = 0, n = 1 and n = 2) through the use of pyrrolidine and tetrathiafulvalene moieties. We applied density functional theory (DFT) methods to determine their electronic properties, linear and nonlinear optical response properties along with their respective UV–Visible spectra using CAM-B3LYP functional and 6-31G* basis set. The isotropic polarizability (α_{iso}) and anisotropic polarizability (α_{aniso}) of 2c was found to be 131.52×10^{-24} and 47.01×10^{-24} esu, respectively. Amongst our designed compounds, the maximum second-order nonlinear optical polarizability amplitude ($\beta_{//}$) of 2c was found to be 15.69×10^{-30} esu. Interestingly, 2c shows the highest third-order nonlinear polarizability amplitude $\langle\gamma\rangle$ of 284.29×10^{-36} esu that is about three times higher than parent compound 1. Additionally, frontier molecular orbitals (FMOs), molecular electrostatic potential maps (MEPs), transition density matrix (TDM) analysis indicate more effective charge redistribution from donor moiety to acceptor fragments. The density of states (DOS) diagrams reveals distinct electronic contributions of various fragments in the formation of HOMO and LUMO orbitals resulting in efficient intramolecular charge transfer (ICT) and robust third-order NLO response properties of functionalized fullerene derivatives. The current study may arouse the attention of the scientific society to utilize the extensive π-conjugation of functionalized fullerenes for designing efficient.

P-05

Research and development on the phytochemistry of Albizia kalkora (Part III)

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Abstract

In continuation of research and development on the phytochemicals of Albiza kalkora we have isolated two new phytochemicals from the methanol extract of the whole plant. The new phytochemicals were finalized as piperidine alkaloids. The structures of the alkaloids were interpreted by the 1D and 2D NMR spectroscopy. UV,

IR and Mass spectroscopy were also the basic part of the elucidated structure. The isolated natural products were evaluated for the thier biochemistry and found that they showed potent inhibitors for cholinesterase enzyme. The plant is also called as Kalkora memosa, belongs to family fabaceae. The morphology of the plant showed that it is medium to large sized tree present all over the world. The branches are dark brown in colour while the flowers are white in colour. In Pakistan it is present from latitude to altitude. The local health practitioners used it's extract for the heart deseases, urinary tract infections and skin deseases. Very little phytochemical work has been done previously on the plant.

P-06

Bioactive Constituents from Echinops echinatus

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Abstract

Echinops echinatus is an important genus of Asteraceae which consist of spiny shrub. This plant is known for its phytochemicals and the promising biological activities. *Echinops echinatus* widely distributed in the tropical and subtropical regions of the world. In Pakistan it is widely distributed from latitude to altitude. In local medicine the plant was used for treatment of lymphangitis, sepsis, trachoma, typhoid, gonorrhea, and ulcerative deseases. The plant is also used to treat respiratory, toothache, leucorrhoea, skin and earache uterine diseases. Literature survey revealed that very less work have been reported from the genus *Echinops*. In the present study phytochemical investigations on *Echinops echinatus* resulted in the isolation of two new ceramic amides along with several known compounds. The structures of isolated compounds were elucidated by the use modern spectroscopic techniques, i.e., EIMS, HREIMS, HRFABMS 1D and 2D NMR and by chemical analysis. The purified compounds were evaluated for their enzyme inhibition studies against lipoxygenase, chymotrypsin and tyrocinase. The two new compounds showed potent inhibitory activities.

P-07

Biologically active constituents from *Hypericum oblongifolium*

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Abstract

Natural Products have gained importance in pharmaceutical industries during last decade due to harmless effects on human health. Many Biological properties associated with Hypericum oblongifolium has been reported in literature. So, this project was designed to investigate biologically active constituents that are hidden in H. oblogifolium. The research led to the isolation of a new triterpene along with three known compounds from chloroform soluble fraction of H. oblogifolium. These compounds were characterized using various spectroscopic techniques including 1D, 2D NMR and mass spectrometry. The structure of new compounds was elucidated as 21β-hydroxy-12-ene-ursane-28-oic acid (1) while known compounds were named as 7,4'-Dihydroxy-5,3-dimrthoxy flavanone (2), α-D-Glucopyranosyl-6'-O-hexadecanoate (3) and Quercetin-3'-O-ß-D-glucopyranoside (4). All these isolated compounds were tested for their antimicrobial and lipoxygenase inhibiting activity. All exhibited moderate to good activity when compared with standard drugs.

P-08

Synthesis of bimetallic cobalt ferrite nanocatalyst and study of their ability for the decomposition of organic pollutants

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Abstract

Bimetallic nanoparticles are considered as efficient catalyst for the decomposition of organic pollutant. Here, bimetallic cobalt ferrite ($CuFe_2O_4$) nanoparticles have been synthesized in aqueous medium. Cobalt chloride ($CoCl_2$) was used as a precursor of copper and ferric chloride ($FeCl_3$) was used as a source of iron. Oleic acid was used as a surfactant during synthesis. UV-VIS and FTIR spectrometric techniques have been employed for characterization of cobalt ferrite nanoparticles. Catalytic ability of the prepared nanocatalyst has been studied by the reduction of organic pollutants (methylene blue and Methyl orange). Results obtained through this catalytic study encourage the use of these bimetallic nanoparticles as catalyst to decompose organic pollutants. The apparent rate constant (k_{app}) values showed the pseudo first order kinetic reaction for the catalytic reduction of pollutants.

P-09

Silver loaded alumina (Ag-Al_2O_3): An effective visible light active photo catalyst for aqueous phase degradation of methylene blue dye

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Abstract

Visible light induced photo catalytic degradation of dyes is an inviting approach in wastewater treatment techniques. In this study, silver loaded alumina (Ag-Al_2O_3) is used as catalyst for aqueous phase photo degradation of methylene under visible irradiation. Ag nanoparticles were immobilized on Al_2O_3 by facile green methods using leaves aqueous extract of *Azadirachta indica.* Advanced characterization techniques like particle size distribution, XRD, TGA, EDX and SEM were used for characterization of as prepared Ag-Al_2O_3 particles. The prepared Ag-Al_2O_3 was tested as catalyst for degradation of methylene blue under visible irradiation. Ag-Al_2O_3 showed improved photo catalytic performance for the degradation of methylene blue dye in aqueous medium. Effect of various parameters on catalytic activity were investigated. Curve Expert computer program was used for kinetics analyses of the data according to Eley-Rideal and Langmuir-Hinshelwood mechanism. A 100 mgL^{-1} solution (50 mL) completely degraded in 120 minutes of reaction duration at 50 °C over 0.1g of Ag-Al_2O_3 as catalyst.

Keywords: Al_2O_3; *Azadirachta indica*; Methylene blue; Langmuir-Hinshelwood; Eley-Rideal

P-10

Determination of selected metals in orange (citrus) fruit

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Abstract

Orange (Citrus Sinensis) is a citrus fruit belongs to the Rutacease family including kinnow, mausami, red blood, grapefruit; succri along with mandarin and total production of citrus fruits in Pakistan is about 37%. The aim of the present study was to determine the selected metals (Cd, Ca, Co, Cu, Fe, Mg, Mn, Pb, Zn and Sr) in orange (Citrus) fruit due to their effect in the human body. The fruits were purchased from different markets. To prepare the laboratory samples, each fruit was cut into slices and crushed the dried samples by chopper. The samples were digested by way of HClO 4 and HNO 3 with ratio (1:4). Selected metals (Cd, Ca, Co, Cu, Fe, Mg, Mn, Pb, Zn and Sr) were measured in the different varieties (mausami, kinnow, succri and red blood) of orange fruit, by atomic absorption spectrophotometer (Shimadzu AA-670, Japan). Significant differences in metal content between the varieties of orange were found. Mean concentrations of Ca, Mg, Zn, Fe and Sr were found to be significantly higher in mussami, red blood, Kinnow and Succri. Comparative distribution of Mn, Cd and Cu higher in red blood orange (Citrus), Ca, Pb and Sr were higher in succri. Comparative distribution of Fe higher in mussami and Mg and Zn higher in kinnow. Obtained results were compared with acceptable levels set out by

WHO. The higher correlation values were observed in case of Pb-Fe, Pb-Ca, Pb-Mg and in Ni-Co that indicates mutual variations in orange varieties. The correlation study revealed significantly diverse relationships among the metals in orange (citrus). Similarly, disparities in the metal concentrations were also exhibited in different types of orange (mussami, red blood, kinnow and succri). The study evidenced considerably divergent variations in the metal levels in different varieties of orange fruit in comparison with the standard solutions.

Keywords: Metal; Orange Citrus; varieties; AAS; Statistical Analysis; Pakistan

P-11

Heat flow in a 2D slab: A MATLAB based estimation

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Abstract

This paper reports the estimation of a basic phenomenon of nature heat flow by solving a set of equations. The flow taken here is two dimensional and the third dimension is intentionally neglected for a simpler calculation. To analyze the heat transfer from its surroundings, a 2D rectangular slab of any material, is divided into a grid (of any desired size i.e. n x n), and then to find the heat flow through grid, Laplace's equation for heat flow is employed. The calculations involve numerous differential equations and their huge iterations for solutions, it's not possible to figure out the results manually for large grid sizes, a MATLAB code for the problem is developed to estimate and visualize the temperature variations and transfer of heat at different points of the grid on the slab, whereas the effect of grid size on estimation of heat flow is also discussed.

P-12

Essential oil constituents from leaves of wedelia

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Abstract

This study provides the chemical profiling of leaf essential oil of wedelia, a plant specifically known for its medicinal uses against epilepsy, fever, headache, sore throat, hepatitis wounds and cold. The extraction was performed with the help of distillation technique. The separation and identification of essential oil constituents were performed through gas chromatography mass spectrometry and 13 compounds were successfully identified in the essential oil such as β-ocimene, α-caryophyllene, α-farnesene, elemol and methoxybenzene and their semi-quantitative analysis was performed. Most of these are well known active constituents especially against pathogenic bacteria.

Keywords: wedelia, Sphagneticola trilobata, GC-MS, essential oil composition, bioactive components.

P-13

Investigation of Cu-doped zinc oxide Zn1-xCuxO (x = 0.01, 0.02, 0.03, 0.04, 0.05) based nanostructures for the elimination of Methylene Blue dye pollutant under sunlight

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Abstract

Herein, copper (Cu) doped zinc oxide (ZnO) namely Zn 1-x Cu x O (x = 0.01, 0.02, 0.03, 0.04, 0.05) are grown by hydrothermal method for photo catalytic activity. The grown samples were characterized with XRD, FTIR, SEM, UV-vis. The XRD results confirmed the successful doping of Cu ions without altering basic hexagonal structure of ZnO. FTIR results also confirm the presence of metal-oxygen bonds vibration related to Zn-O bonds. UV-vis results showed that the energy band gap decreased with the increase in the doping concentration of Cu. SEM images shows the nano rods type morphology which is improved with the increasing Cu doping.

Photocatalytic activities of all synthesized samples were tested against methylene blue (MB) dye under the sunlight irradiation. The Zn 0.95 Cu 0.05 O photo catalyst show a best photo catalytic activity with 99.9% elimination of MB dye within 60 min, as related to the pure ZnO and 1%, 2%, 3%, and 4% Cu doped ZnO. In comparison to the other catalyst, value of the rate constant for Zn 0.95 Cu 0.05 O was greater than the pure catalysts. The excellent photocatalytic activity of Zn0.95C0.05O is accredited to 1) presence Cu ions that successfully suppress high recombination of electron hole pair which, in turns find the enough time to produce extra reactive species for degradation MB dye and 2) Lower energy bandgap of ZnO by 5% Cu doping in visible region which leads to higher number of electrons excitation from valence band to conduction band. Hence, the present finding introduces a strategy to reduce the energy bandgap of ZnO from UV.

P-14

Monte Carlo modelling of tissue heterogeneity in radiotherapy

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Abstract

At present, the process of simulation has become important technique as in order to minimize the disparity between the calculated dose distribution, phased at treatment planning and those distributed to the patient. It includes EGSnrc based Monte Carlo codes. Linear accelerator head BEAMnrc used for modeling, DOSXYZnrc code utilized for performing dose calculations. Here and now, the study aims at Monte Carlo modelling of tissue heterogeneity in radiotherapy. For this purpose, Nylon-Beryllium (medium1) as a tissue-bone heterogeneity substitute were chosen and percentage depth doses (PDDs) and lateral profiles were achieved for a tissue-bone heterogeneity substitute for the diversity of field sizes and beam energies 6MV and 10MV. Different types of graphs were procured with discrete results, using the above stated techniques for dose calculation. According to the consequences the results suggests that medium1 is equivalent to tissue-bone in the buildup region with both energies.

P-15

SERS for studying interaction of n-propyl substituted imidazole compound with DNA

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Abstract

Imidazole is an organic compound with the formula $C_3N_2H_4$. It is white in color, crystalline in nature and have solubility in water, producing a mildly alkaline solution, its solubility also relates with polar solvents. Because the hydrogen atom can be found on any of the two nitrogen atoms. Five-membered nitrogen containing heterocyclic ring is common in many biological active compounds. In the field of pharmacology, imidazole and its derivatives are widely used as anticonvulsant, antimicrobial, anti-inflammatory, anticancer, analgesic, anti-Parkinson, and anti-HIV activities. The reason why we prefer imidazole compound over other is just because it have interacting capability with DNA and have ability to perceive changes after their interaction. We employ SERS for studying what changes occur after their interaction. SERS which is rapidly establish into an advance analytical tool since 1974. SERS have wide range of applications in research including the formation of inter-strand cross-linking in the double helix of DNA. Different concentrations of the ligand are prepared and mixed with specific quantity of DNA for interaction and SERS spectra are recorded for each solution. Silver nanoparticles are used for the enhancement of Raman signals and as SERS substrate. Moreover, Multivariant data analysis technique like principal component analysis (PCA) and partial least squares-discriminant analysis (PLS-DA) are employed further for detailed study.

P-16

Biosynthesis and Characterization of Ce-Pb bimetallic nanoparticles by using Lantana camara extract for photocatalytic activity

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Abstract

The synergy between two different metals provides a dramatic enhancement in the bimetallic nanoparticles' catalytic properties since bimetallization improves the properties associated with the presence of two individual metals. Cerium-lead bimetallic nanoparticles were prepared fromtheir salts by usingLantana Camara extractthat act as a capping and stabilizing agent. The color change of solution fromyellowish golden to dark brown and absorbance peaks at 232 nm and 344 nm for lead and cerium respectively, confirm the formation of Ce-Pbbimetallic nanoparticles with the help of UV/Visible spectroscopy. Both metals showed the red shift after the formation of bimetallic nanoparticles from 223 nm to 232 nm, and 335 nm to 344 nm for lead and cerium respectively. The structural properties of the photo catalysts were examined by using different techniques, e.i., scanning electron microscopy (SEM), x-ray diffraction (XRD) and energy dispersive x-ray spectroscopy (EDS). These bimetallic nanoparticles showed 71% photo degradation against methyl orange in the presence of sun light.

P-17

Mango Kernal Char as adsorbent, surface area and adsorption studies

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Abstract

Classical method was used for the determination of surface area of the mango seed Kernel char using methylene blue dye as model adsorbate molecule. The adsorption capacity (Q max) was also determined (67.56 mg/g) from Langmuir fit (= 0.902). Two hours contact time was required to establish equilibrium and pH seems to have no much effect on adsorption process. The calculated surface area by adsorption process was found to be 85.19 /g for MSK-600.

P-18

Adsorption of toxic heavy metals from waste water by using magnetic nickel and cobalt-doped nickel ferrites

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Abstract

Water is the main constituent of all kind of living organisms. Due to industrialization and urbanization, contamination of water was increased day by day. The concentration of the heavy metals beyond a certain level has dangerous impact for human health and surrounding environment. Therefore, there was an urgent need for the nanotechnology to provide new treatments for the purification of water from hazards pollutants. Nanotechnology was introducing the magnetic ferrites that were effective in this respect. Magnetic ferrites were prepared by co-precipitation method, with high specific area and adsorption capacities were operative for the elimination of heavy metals from contaminated water. Nickel and cobalt-nickel Nano composites were manufactured for the extraction of heavy metals such as Cu, Ni, Co, Zn and Mn from wastewater. Ferrites having best adsorption qualities were characterized using XRD, FT-IR, UV-visible spectroscopy and SEM. These nano ferrites were applied as nanoadsorbant for removing of several toxic metals. The nanoadsorbant were bounded with the heavy metals and filtration was used for the extraction of these metals. (AAS) was used to determine the percentage removal efficiencies of ferrites. The percentage adsorption efficiencies of Zn, Ni and Mn by using the Nickel ferrites was found to be 85 %, 87 %, and 98 % respectively. The adsorption percentage of Zn, Co, Ni, and Mn with the Cobalt-nickel ferrites was calculated as 23 %, 34 %, and 52 % respectively. The experiments were

repeated many times with same parameters and the results are obtained as Nickel magnetic ferrites are exhibiting the greater efficiency as compare to the Cobalt doped Nickel magnetic ferrites.

P-19

Sintering effect on structural, optical, and electrical properties of cobalt doped tin oxide nanostructures

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Abstract

In this work, a quick chemical approach was used to prepare tin oxide nano powder by doping cobalt. Cobalt-doped SnO2 nanoparticles were manufactured by the sol-gel technique. The sintering effect on structural, optical, and electrical properties of synthesized nanostructures was investigated. X-ray diffraction was performed to analyze the structure and crystallite size of developed nanoparticles. Morphology and particle size of produced nanostructures were evaluated utilizing scanning electron microscopy. Raman spectroscopy was conducted for the optical behavior of created samples. Furthermore, electrical properties were examined for the calculation of resistivity and conductivity of fabricated samples using two probe method. It is hoped that such type of desired material could be utilized in optoelectronics and microelectronics fields of interest.

P-20

Bioassay –Guided Isolation and GCMS Analysis of Malvastrum Coromandelianum (L.) Garcke and Curcuma zedoria Roxb

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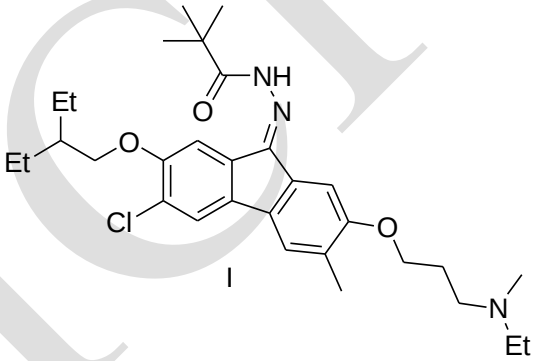
Abstract

Malvastrum coromandelianum (L.) Garcke, an invasive alien weed, is of immense pharmacological value. Two major Phytoconstituents, Substituted Azide (I) and diterpenes (II), have been identified from the ethyl acetate sub-fraction of 80 % methanol crude extract of the aerial parts of *M. coromandelianum via* GCMS along with 20 other bioactive compounds, categorized under sterols, terpenes, phenols, vitamins, flavonoids, fatty acids, which have shown significant microbial activities against *E. coli, C. albicans, S. aureus.* The plant species may serve as a natural resource for potential antioxidant molecules, it being a source of phenols with high radical scavenging ability



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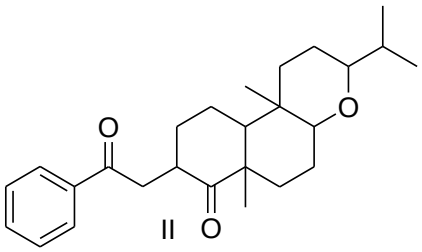
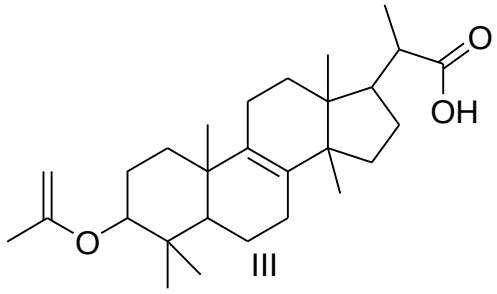


II

Zedoaria (*Curcuma Zedoaria* Roscoe Zingberaceae) is a perennial herb commonly known as white turmeric. A sesquiterpenes, 2-(2-acetoxy-4.4.14-trimethylandrost-8-en-17-yl was identified via GCMS from the bioactive fraction of the methanolic extract of fresh rhizomes of *C. zedoaria* which has shown significant activities such as antimicrobial, antioxidant, and cytotoxic. The finding of our research confirmed the medicinal value of selected plants and other complementary uses making them doubly attractive for incorporation in commercial-scale studies for the development of primary health care systems.



2-(2-acetoxy-4.4.14-trimethylandrost-8-en-17-yl)

Keywords: *Malvastrum coromandelianum, Curcuma Zedoaria*, GCMS, Phytochemicals, Anti-microbial, Antioxidants, cytotoxic activity.

P-21

Laser spectroscopy of nanostructures

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Abstract

This study probes the laser-induced plasma of doped and undoped nanostructure. Spatial and temporal evaluations of laser-induced plasma were probed. Tin oxide and Cd doped tin oxide nanomaterials have been synthesized by Co-precipitation. X-ray diffraction (XRD), scanning electron microscope (SEM) and transmission electron microscopy (TEM) techniques were used to verify the nanostructure and morphological properties of doped and undoped materials. In LIBS Nd: YAG laser was used to produce nanoplasma on the surface of the nanomaterial. The temporal evolution of laser-induced plasma of nanostructure is recorded at different incident laser fluences. At the beginning of plasma evolution, a continuum emission dominates the spectrum. With time evolution, the line emission intensity increases with the reduction of the continuous emission. However, the emission line intensities reduce after a certain delay with the cooling down of the plasma. It is hence important to choose a suitable detection time window to detect a specific line with a good signal to continuum ratio. Spatial and temporal variations of Sn and Cd atoms and ionic excited atoms were reported. Light emitted from plasma gives plenty of information about the samples and also helps to find the plasma parameters. Spatial and temporal distributions of nanoplasma were compared with plasma distribution bulk material.

P-22

Structural, thermal and magnetic properties of Al_3^+-doped nanostructured spinel nickel-cadmium ferrites

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Abstract

Aluminum–nickel-cadmium ferrite nanostructure with a nominal composition of Ni0.6Cd0.4Fe2-x AlxO4 (x=0.1, 0.2, 0.3 and 0.4) was synthesized by hydrothermal process. The effects of Al_3^+ substitution on structural, quantitative, qualitative and magnetic properties were characterized via X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX) and vibrating-sample magnetometry (VSM). XRD and EDX characterization of the samples revealed a single-phase inverse spinel structure and decrease in average crystal size as Al concentration increases. The decrease in average crystal size as Al_3^+ ions content increases is associated with structural effects of overall crystal size of nanostructure. The development of a thermally stable nickel-cadmium ferrite above 600 °C was detected by thermogravimetric

analysis (TGA) measurements. The magnetic hysteresis loop measurements at room temperature (RT) with an ultimate tested magnetic field of 2.0 T shows both saturation and remnant magnetization decrease as content of Al_3^+ ions substitution increases. The decrease in overall magnetization is due to spin non-collinearity, weakening of magnetocrystalline anisotropy and weak super-exchange interactions.

P-23

A DFT approach for finding therapeutic potential of two dimensional (2D) graphitic carbon nitride (GCN) as a drug delivery carrier for curcumin to treat cardiovascular diseases

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Abstract

DFT analysis is used to predict the therapeutic potential of GCN as a medicinal carrier for curcumin for the treatment of cardiovascular diseases. To evaluate the drug transport capacity of GCN, the electronic, ground, and excited-state properties of curcumin, GCN, and the GCN-curcumin-complex were investigated. The adsorption energy of the GCN-curcumin-complex is higher in the gas phase (-0.25eV) than in the aqueous phase (-0.09eV), implying that the GCN-curcumin-complex is more stable in the gas phase. Weak N-H bonds anchored the curcumin at GCN surface. The GCN-curcumin-complex has a higher dipole moment in the aqueous medium (2.37 D) than in the gas phase (1.36 D) which aids in the efficient transport of the drug through biological systems. Molecular electrostatic potential and frontier molecular orbitals revealed that during excitation, curcumin behaves as a HOMO, transferring charge to the LUMO (GCN). The charge decomposition analysis, which determines the highest overlap between the curcumin and GCN orbitals, was also employed to investigate the charge transfer process. For several transitions from the donor to the acceptor, NBO analysis revealed that charge was transferred between the curcumin and GCN molecules. For the GCN-curcumin-complex, excited-state calculations show that λmax is redshifted by 131 nm. The redshift for the GCN-curcumin-complex in the solvent phase is 149 nm. The theoretically generated spectra match experimentally observed spectra quite well. Moreover, the in silico infrared spectra of GCN and Curcumin is also close to the experimental spectra. For the graphical explanation of various excited states, electron-hole and photoinduced electron-transfer analysis are performed. The PET mechanism perceives quenching of fluorescence because of an interaction. Moreover, GCN +1/-1 showed little structural change and produces stable curcumin complexes. All findings indicated that GCN has substantial therapeutic potential as a carrier for curcumin in cardiovascular disease cure. Researchers will be motivated to investigate alternative 2D nanomaterials for drug delivery applications due to this theoretical study.

P-24

SERS for characterization of supernatant of biofilm forming bacterial strains

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Abstract

The generation of adherent, multilayered bacterial biofilms is the most important factor in the development of infections that commonly fail to respond to effective antibiotic treatment. Biofilm-forming microorganisms are linked to chronic and recurring human diseases and are extremely resistant to antibiotics. The technique of a study on a major problem in microbiology laboratories, the difficulty in differentiating Staphylococcus genus strains, is described. In the current study, surface enhanced Raman spectroscopy was used to identify and characterise various strains of Staphylococcus epidermidis supernatant (non-biofilm forming, medium, and strong biofilm-forming bacteria). Silver nanoparticles (Ag-NPs) were used as the SERS substrate and they were synthesized using a chemical reduction process. The bacteria Staphylococcus epidermidis has emerged as a common cause of nosocomial infections. Staphylococcus epidermidis is a Gram-positive bacterium that belongs to the Staphylococcus genus, which has around 40 species. Its capacity to build biofilms on indwelling medical devices is mostly responsible for its pathogenicity. S. epidermidis is protected from immune system attacks and antibiotic

therapy in biofilms, making S. epidermidis infections difficult to eradicate. The SERS spectral features of these centrifuged supernatant samples were examined using multivariate statistical techniques such as Principal Component Analysis (PCA) and Partial Least Square Discriminant Analysis (PLS-DA). Different centrifuged samples were distinguished using PCA. Furthermore, the PLS-DA technique was used to differentiate and classify centrifuged supernatant samples. Receiver operating characteristic (ROC) curves, goodness of fit (R2), and prediction accuracy were all factors in the PLS-DA model.

P-25

Application of raman spectroscopy for qualitative and quantitative analysis of pharmaceutical products (azithromycin)

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Abstract

Commercial formulation of pharmaceutical products is a modern-day requirement and qualitative and quantitative control of drug components is far more important aspect of quality control process in pharmaceutical industry. A Pharmaceutical drug consist of two components, API and Excipients. Analysis of both these components is compulsory as a minor variation in concentration or impurity can cause serious damages. Raman Spectroscopy is an emerging technique which can be use for qualitative and quantitative analysis of substances with little or no sample preparation. In this study we will record Raman spectra of different dosage forms of Azithromycin (an antibiotic) with self-made concentrations of API and Excipients and will develop a modal with the help of self-developed protocols in Matlab Software. We will use PCA and PLSDA protocols for qualitative and quantitative analysis respectively. We will also analyze commercially available dosage forms of Azithromycin to evaluate performance of our modal. Keywords: Raman Spectroscopy, Azithromycin, Pharmaceutical, Qualitative and Quantitative analysis.

P-26

Raman spectroscopy for the analysis of solid dosage forms of Rosuvastatin

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Abstract

In recent times, industrial progress requires more accurate tools and a more rapid analytical method that can be set up to determine the effectiveness of drugs. As in the modern era, Raman spectroscopy is emerging for the analysis of solid state drugs because it is a fast and non-invasive method. Raman spectroscopy is widely employed in various industries, such as the food and dye industries. The great advantage of Raman spectroscopy is that it does not require sample preparation. In addition, it will be used for aqueous solutions. Raman spectroscopy can be used to analyse solid dosage forms of pharmaceuticals in both qualitative and quantitative ways. To compensate for the commercially available drug formulations, various concentrations of solid dosage forms of drugs will be developed. A principal component analysis (PCA) model will be employed for qualitative analysis. In addition, a partial least square regression analysis will be used to evaluate the relationship between the various concentrations of active pharmaceutical ingredients (APIs) and excipients. The results of this study will provide the most effective and reliable identification and analysis of active pharmaceutical ingredients in solid dosage forms and, at the same instant, will make Raman spectroscopy a powerful alternative tool for such purposes, even on a large industrial scale.

Keywords: Rosuvastatin; raman spectroscopy; API; Excipients

P-27

SERS for studying interaction of n-propyl substituted imidazole compound with DNA

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Abstract

Imidazole is an organic compound with the formula $C_3N_2H_4$. It is white in color, crystalline in nature and have solubility in water, producing a mildly alkaline solution, its solubility also relates with polar solvents. Because the hydrogen atom can be found on any of the two nitrogen atoms. Five-membered nitrogen containing heterocyclic ring is common in many biological active compounds. In the field of pharmacology, imidazole and its derivatives are widely used as anticonvulsant, antimicrobial, anti-inflammatory, anticancer, analgesic, anti-Parkinson, and anti-HIV activities. The reason why we prefer imidazole compound over other is just because it have interacting capability with DNA and have ability to perceive changes after their interaction. We employ SERS for studying what changes occur after their interaction. SERS which is rapidly establish into an advance analytical tool since 1974. SERS have wide range of applications in research including the formation of inter-strand cross-linking in the double helix of DNA. Different concentrations of the ligand are prepared and mixed with specific quantity of DNA for interaction and SERS spectra are recorded for each solution. Silver nanoparticles are used for the enhancement of Raman signals and as SERS substrate. Moreover, Multivariant data analysis technique like principal component analysis (PCA) and partial least squares-discriminant analysis (PLS-DA) are employed further for detailed study.

Keywords: Imidazole, DNA, Silver nanoparticles, SERS

P-28

Surface enhanced raman spectral characterization for monitoring the antibacterial activity of hexamine salt

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Abstracts

In treatment and prevention of different diseases quantification of antibiotics is of significant importance. For efficient antibacterial drug, definite basic properties are assigned. For minimization of side effect in humans these are mostly designed to act distinctively, uniquely and selectively against bacterial strains. For the drug to reach the infectious site selectively it must be able to enter human tissues. To determine the minimum inhibitory concentration (MIC) for bacterial strains like Streptococcus agalactiae and Escherichia coli against hexamine salt to check inhibition zone Muller-Hinton Broth (MHB) dilution method will be used. In the ongoing study, hexamine salt sensitive to bacterial strains, its differentiation and identification will be characterized through SERS by using Ag NPs as a SERS substrate. The cell wall components of bacterial body in SERS characterization related to vibrational mode of nucleic acid (727cm^{-}1), Protein (835-825cm^{-}1), Carbohydrate (554cm $^{-}$1) and Lipid (1181cm $^{-}$1). Through Chemometrics tools like Principal Component Analysis (PCA) and Partial least square-discriminate analysis (PLS-DA) the SERS spectral features of the antibacterial samples will be analyzed. PCA transform largely correlated variables into smaller number of uncorrelated variables by reducing dimensionality. Partial Least square discriminate analysis (PLS-DA) is a classification model was employed for the discrimination.

Keywords: Antibacterial activity, Hexamine Salt, SERS

P-29

Surface-enhanced Raman spectroscopy (SERS) for analysis of adulterated pesticide samples of Pyriproxyfen

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Abstract

Pesticides are essential in modern agricultural practices. Fake pesticides are being sold illegally all over the world. Adulteration of pesticides can occur at any level of the production process, including when substandard raw materials and low-quality solvents are used to generate the ingredients (AI) or the formulation, as well as when needed purification operations are skipped, resulting in contaminants. Due to expiration, reduced active chemical, and excipient interaction, original insecticides can lose their potency. Adulterated pesticides are a big problem in Punjab and Sindh cotton belts. Pyriproxyfen was detected and characterized to µg/L using surface-enhanced Raman spectroscopy (SERS) technique. To serve as a test surface for SERS, tiny layer of silver was placed to nanoscale substrates. AgNPs were characterized using Dynamic Light Scattering (DLS) and a scanning electron microscope (SEM). SERS, a quick detection device, was used to identify pesticides at ppm quantities. Statistical analysis by Partial Least Square Regression (PLSR) and Principal Component Analysis (PCA) will be used to differentiate between adulterated pesticides from the original ones. In terms of accurate, quantitative pesticide detection, the proposed, the proposed technology appeared to be highly promising, and it could be applied to a wide range of agricultural products as well as other areas of food science.

Keywords: Adulteration, silver nanoparticles, active ingredient, impurities.

P-30

Detection of Ethyl methane-sulfonate adulterant in organophosphate insecticide through Surface-enhanced Raman Spectroscopy (SERS)

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Abstract

Malathion is a member of organophosphate insecticide and widely used for control of insect pests of vegetables and other agricultural crops. Adulterated pesticides are very common in market now-a-days. Such types of pesticides are not effective at all and also dangerous to human health. Malathion mostly adulterated at the stage of manufacturing of active ingredient and also at the at the time of preparing formulation. Ethyl methane-sulfonate (EMS) as an impurity present in malathion at high level such as 30 ppm which has mutagenic teratogenic and potentially carcinogenic effect. For this substance, the promising limit are estimated at 0.1 ppm. Therefore, current research work was planned to investigate the different concentration of the adulterant present in pesticide by using Raman Spectroscopy coupled with silver nanoparticle. nanoparticle used for enhanced the surface. The prominent peaks in adulterated pesticide were 785,1282 and 1029 cm -1 due to this adulterant which were absent in pure pesticide, formulation. SERS features further analyzed through Principle Component Analysis (PCA). For quantification of the adulterant, Partial Least Squares Regression (PLR) was performed. Peak intensity was found directly linked with concentrations of the adulterant. Hence, such techniques are effective for the detection of adulterant up to its promising limit also distinguish the adulterated and pure pesticide.

P-31

Raman spectroscopy for the of solid dosage forms of pharmaceutical drug Febuxostat

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Abstract

Raman spectroscopy is an analytical technique progressively employed to demonstrate its potential in the determination of solid dosage forms of pharmaceutical drugs. Numerous analytical techniques have showed their potential in qualitative and quantitative analysis. But those techniques are much laborious and requiring more experience for analysis. In this modern era, the need of the time is to use highly sensitive and less time-consuming technique in which no sample preparation is required and Raman spectroscopy is found to be successful in pharmacy for estimation of solid dosage forms due to its proper functionalities. In this context, estimation of solid dosage form of Febuxostat will accomplish by making different formulations. Principle component analysis,

Partial least square regression analysis and regression model in wavenumber range of 200-1800cm -1 was applied for the classification of different Febuxostat formulations, quantification of unknown self-made sample and to check the reliability of planned method. Furthermore, root mean square (RMS) error of calibration, prediction and coefficient of determination (R2) was found to be 2.9, 1.35 and 0.99.

Keywords: Febuxostat; raman spectroscopy; API; Excipient; RMSEC; RMSEP

P-32

Raman Spectroscopy for the analysis of Pharmaceuticals (METFORMIN)

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Abstract

Drugs and associated precursors need to be monitored qualitatively and quantitatively in the pharma industry, especially during the drug discovery and development process. Various analytical techniques, such as high-performance liquid chromatography (HPLC) and thin-layer chromatography (TLC), are utilized in this regard, notably spectroscopic ones. In this aspect, Raman spectroscopy has a good prospect for such applications since it requires little to no sample preparation. Metformin, an important antidiabetic medication, is investigated using Raman spectroscopy and multivariate data analysis approaches in the ongoing work. The Raman spectra of Metformin are being used to explore the drug's molecular vibrations to propose a reliable method based on Raman spectral features used for the analysis or drug. Multivariate techniques such as Principal component analysis (PCA), Linear discriminant analysis (LDA), and Partial least square regression (PLSR) are used to evaluate drug Raman spectra using MatLab. In the critical spectral range of 50–1700 cm -1 , it is established that very narrow (4–10 cm -1) spectral lines of molecular vibrations are found in the metformin hydrochloride pressed powder sample. These can be used to determine which chemical bonds create spectrum components corresponding to specific functional group vibrations. Raman Spectroscopy has a tremendous promise for non-invasive detection of anti-diabetic drugs.

Keywords: Raman Spectroscopy, Metformin, Partial least square Regression

P-33

Surface enhanced Raman spectroscopy for coal biodesulfurization of thiophene compounds by bacterial sp.

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Abstract

Biodesulfurization is found to be quite efficient in removing thiophene compounds from coal or petroleum products. Sulphur-containing compounds are chief cause of environmental problems globally. Desulfurization through microbes is both eco-friendly as well as cost-effective. For this purpose, bacterial sp. will use to desulfurize S-compounds to make sulphur-free coal. Surface Enhanced Raman Spectroscopy is considered as novel technique for the analysis of active removal of sulphur contents from coal. Several spectral peaks will show the concentration of thiophene compounds, then be pre-processed using MATLAB 7.8. In data pre-processing, various steps viz., substrate removal, baseline correction, vector normalization and smoothening will be used. SERS spectral acquisition using PCA and PLS-DA will prove to be effective in biodesulfurization of thiophene compounds.

Keywords: Biodesulfurization, thiophene compounds, SERS

P-34

Synthesis of functionalized 5-bromothiophene-2-carboxylates and anti-bacterial studies

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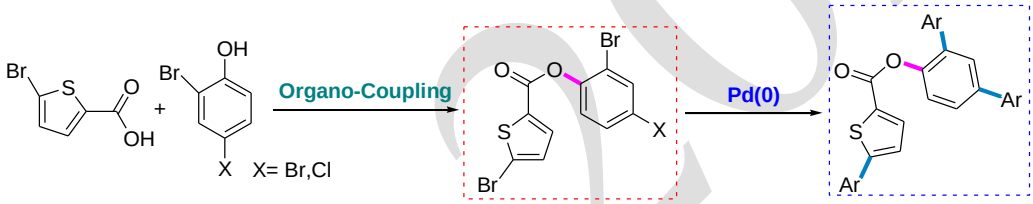
Abstract

Thiophene based therapeutics have shown antibacterial, and broad spectrum of activities. Herein, the 2,4-dibromophenyl-5-bromothiophene-2-carboxylate and 2-bromo-4-chlorophenyl-5-bromothiophene-2-carboxylate were produced through Steglich esterification of 5-bromothiophene-2-carboxylic acid with 2,4-dibromo phenol and 2-bromo-4-chlorophenol. Suzuki cross-coupling is an essential reaction in industries and labs for combinatorial and synthetic reasons from a synthetic perspective. Both stereo-selective and region-selective products may be obtained by using this coupling. The Suzuki-Miyaura cross-coupling process catalyzed by Pd(0) was employed to produce 2,4-biarylphenyl-5-arylthiophene-2-carboxylate and 2-aryl-4-chlorophenyl-5-aryl thiophene-2-carboxylate derivatives in moderate to good yields in this work. Binding interactions of all produced compounds with MurD and MurE *Escherichia coli* proteins were theoretically examined by molecular docking studies, suggesting strong binding affinities, to screen out the most active lead compounds. The structural and reactivity characteristics were estimated using DFT-B3LYP/3-21g and DFT computations. Major obtaining compounds have shown potential reactivities and charge distributions, indicating that they are effective against biological targets. Based on theoretical conclusions, these compounds were evaluated in vitro for antibacterial activity against Gram-negative bacteria (*Escherichia coli*) at various doses. The 5-chloro-3',5'-difluoro-[1,1'-biphenyl]-2-yl5-(3,5-difluorophenyl)thiophene-2-carboxylate was determined to have the greatest potential value, strongest binding affinities, and a promising antibacterial agent with a MIC value of 50 mg/ml against *Escherichia coli*.



P-35

Quantitative detection of pesticide (Emamectien benzoate) based on SERS

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Abstract

One of the world's major food safety concerns is the pesticides in fruits and vegetables. Pesticide detection is a seminal step in regulating and monitoring pesticide levels in the environment. Although GC/LC-MS is often the traditional method for pesticide detection, these methods are typically complicated, time-consuming, and costly. Recently, Raman spectroscopy in conjunction with silver nanoparticles (SERS) was used to create a fast, low-cost, and subtle method for qualitative and quantitative analysis of trace levels of pesticide emamectien benzoate. The Raman spectra of Emamectin benzoate were obtained using AgNPs as surface enhancers and Raman shifts of 686cm -1 as the peaks of interest. This peak intensity was concentration-dependent; the higher the concentration, the greater the Raman shift. Principal component analysis (PCA) will be used to further evaluate SERS spectral features. The partial least squares (PLS) model will be used to detect emamectin benzoate quantitatively. In terms of precise and reliable quantitative pesticide detection, the proposed method looks very promising, and it could be applied to a wide range of agricultural products and many other areas of food science.

P-36

Application of SERS for mutated enzymes produced by *Aspergillus niger*

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Abstract

Aspergillus niger, haploid ascomycete is a common fungus found in nature which produces several important enzymes. In biotechnology and other industries, these enzymes such as protease, cellulose, glucoamylase and amylase play an essential role. Mutations can improve enzyme activity, allowing small amounts of enzymes to synthesize more products. The goal of this study is to use Surface Enhance Raman spectroscopy to study the A. niger mutated enzyme. Surface Enhance Raman spectroscopy is able to analyze these enzymes on the basis of intra-class (between genetically altered enzymes) and inter–class (between unmutated and mutated enzymes) differences. To evaluate the validity of the SERS spectral characteristics, multivariate data analysis statistical methods such as PCA and PLSDA will be used. These statistical tools may distinguish SERS spectral information based on biomolecular changes. PCA, on one hand, provides qualitative data, whereas PLSDA on other hand may quantitatively separate SERS Spectral data.

Keywords: *Aspergillus niger*; Enzymes; Mutations; SERS; PCA; PLSDA

P-37

Raman sepectral characterization of mono azolium salt with butyl substitution and its silver acetate complex through n-heterocyclic linkage

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Abstract

Silver 1-N- heterocyclic carbene complexes are the most popular in organometallic chemistry for their immense utilization in various field like catalysis transmetallation, pharmaceutics and dye sensitization solar cells. In the field of organometallic chemistry, N-Heterocyclic carbenes (NHCs) are considered to be most illustrious and fascinating class of organometallic compounds with well-known complexes. The NHCs interact with the metals centers primarily through strong σ-donation and weak π acceptor properties and therefore results in stable metal complexes. These ligands show advance development in the anticancer and antibacterial activity and have vast importance in the medical field. NHC ligand show high stability and consider as transition metal complex. For the characterization of organometallic complexes and silver complexes we employed a technique the technique used for their characterization is Raman, that is considered as one of the more efficient techniques and have great significance in biological field. Raman spectroscopic analysis have been done in our present research work. Specific amount of the ligand will be taken on the aluminum slide and spectra will be recorded at different focuses. Raman spectrophotometer with Peak Seeker Pro_785: Aileron, USA will be used for analysis. The results obtained will be further processed via Matlab software 7.8 (Mathworks, U.S.A). Principal components analysis (PCA) will be employed for further analyzing the Raman spectral features of organometallic ligands and its Ag complexes. As PCA helps to reduces the dimensionality and increase variability between ligand from its complex

Keywords; organometallic, Carbene complexes, ligand, Raman spectroscopy

P-38

SERS spectroscopic analysis of RNA samples of different subtypes of Hepatitis C

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Abstract

Hepatitis C is a transmittable and dangerous liver disease that is caused by the HCV virus. If this infectious disease is not treated earlier then it can become chronic and eventually lead to hepatocellular carcinoma and liver cirrhosis that can consequently result in death. In the present study, surface-enhanced Raman spectroscopy (SERS) will be employed for the analysis of RNA samples of different subtypes of Hepatitis C (HCV) infected patients and compared them with that of healthy ones. SERS spectral characteristics will be determined in the subtypes of Hepatitis C and increased viral loads will be considered as the SERS spectral biomarkers for HCV infection. For convenience, several levels of these viral loads will be categorized as a low, medium, high and negative control. To check the effectiveness of the SERS for the distinction of the spectral datasets of different

samples of changing viral loads of the healthy as well as unhealthy persons, PCA (principal component analysis) will be applied that is used to compare these subtypes of HCV which includes different intensities of these viral loads with one another and also with that of healthy ones. Furthermore, partial least square discriminant analysis (PLSDA) and partial least square regression analysis (PLSR) will be used for sorting of different viral loads in the HCV positive samples, also the prediction of viral loads of the unknown samples. PLSR model is valid for the prediction of an unknown sample.

Keywords; HCV subtypes; silver nanoparticles; SERS; Genotypes of Hepatitis C; PCA, PLSDA, PLSR

P-39

Raman Spectral Characterization of Antifungal Activity of Organic Salt

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Abstract

Antifungal agents are routinely used to treat pathogenic fungus, although certain fungal strains have developed resistance to antifungal medicines in various ways, which may lead to economic loss over the World. Many Fungi are resistant to Organic salts having Imidazolium derivatives, which are employed as antifungal agents in clinical laboratories. In the present investigation, Broth microdilution method will be used to estimate the minimum inhibitory concentration (MIC) of Imidazolium salt in opposition to two fungal species. Surface Enhanced Raman Spectroscopy (SERS) will be operated to identify the antifungal activity of different concentrations of Imidazolium salt over fungal strains. SERS Spectral data based on fungi inoculated with different drug concentrations will be analyzed qualitatively by using chemometric technique named principal component analysis (PCA). The rapid and sensitive Surface Enhanced Raman spectroscopy would be proved an alternate work for getting comprehensive results with low sample preparation and low cost in medicinal chemistry.

Keywords: Antifungal activity, Imidazolium derivatives, SERS

P-40

Raman spectroscopy for the quantitative analysis of pharmaceutical drug (lornoxicam)

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Abstract

Raman spectroscopy is a powerful analytical tool that is increasingly used in the pharmaceutical industry to analyse solid-state pharmaceutical drugs. The potential of Raman spectroscopy for the qualitative and quantitative analysis of solid dosage pharmaceutical formulations is demonstrated by describing different concentrations of Lornoxicam. For this purpose, different formulations of Lornoxicam were prepared. The increase in API concentrations induces all of the chemical changes in the Raman spectral features associated with the drug and excipients. Changes in the Raman spectral features of API and excipients in Lornoxicam solid dosage forms were investigated using a detailed review of the literature, and their Raman peaks were assigned. The spectrum responses were analysed qualitatively and quantitatively using Principal Component Analysis (PCA) and Partial Least Squares Regression (PLSR). A PLSR model is designed that allows for the prediction of various drug concentrations in complex excipient matrices. The Root Mean Square Error of Cross Validation (RMSECV) was determined to be 1.46 mg during the development of the prediction model, and the variability described by the model, according to the (R2) value, was found to be 0.99. Furthermore, the API concentration in the unknown sample was measured. In comparison to 15/35 mg (w/w), this concentration was predicted to be 14.13/35 mg (w/w). These findings suggest that using lab-built calibration models, Raman spectroscopy combined with PLSR analysis is a reliable tool for determining Lornoxicam content in pharmaceutical samples.

Keyword: Raman spectroscopy, Lornoxicam API, Excipients, Peak assignment, MATLAB

P-41

SERS Analysis of Biodesulphurisation of benzothiophene by supernatant bacterial culture

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Abstract

Microorganisms are metabolically versatile and capable of converting almost every identified group of chemical compounds found in coal into a variety of forms. Biodesulphurisation [cleavage of the carbon–sulfur (C–S) bond) of thiophenes compounds such as Dibenzothiophene (DBT) the most abundant type of organic sulphur found in fossil fuels. It is one of the key microbial metabolic activities in the environment. In the current investigations, newly identified bacterial isolates from the genera Gordonia enriched from various samples, in the presence of DBT as the only source of organic sulphur will be analyzed. The SERS analysis of Dibenzothiophene grown bacterial cultures will be shown the DBT consumption as well as growth of 2-hydroxybiphenyl (2-HBP). SERS analysis will be done by using Ag-nanoparticles synthesized by using chemical reduction method. SERS spectral features of the supernatant bacterial cultures will be further investigated by using multivariate statistical tools such as principal component analysis (PCA) and partial least square-discriminate analysis (PLS-DA).

P-42

Raman spectroscopy for the quantitative and qualitative analysis of solid dosage forms of Salbutamol

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Abstract

Drug development is always an encouraging step to enhance the quality and standard of life by developing medicines against diseases. The modern era of industrialization demands an ultra-sensitive method for the direct quantification of drug API in solid dosage forms. Inhalable medicines that are commonly employed for the treatment of respiratory disorders like salbutamol and salmeterol. Previously, different analytical techniques such as gravimetric and volumetric have been applied for monitoring salbutamol drugs but, these techniques are destructive and time-consuming for analysis. So, Raman spectroscopy will be employed for the quantitative and qualitative analysis of salbutamol drug. Principal component analysis (PCA) and partial least square (PLSRA) regression analysis will carry out for monitoring the quality as well as quantity of the different formulations of salbutamol drug. The results of this study will provide an effective and very reliable identification and quantification of salbutamol API in solid dosage forms.

Keywords: Raman Spectroscopy; pharmaceutical drug; Salbutamol; API; PLSR; PCA.

P-43

Raman spectral characterization of Terminal N-Octyl Substituted bis-imidazolium salt and its organoselenium compounds

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Abstract

In the field of organometallic chemistry, N-heterocyclic carbenes (NHCs) are considered to be most illustrious class of coordination compounds for different purposes especially in catalysis and pharmaceutical industry. Due to their facile synthesis and strong σ-donor and weak π-accepter characteristics towards metal they produce stable adducts. In addition, these organometallic compounds have proven to be better in efficacy and produced low cytotoxicity as compared to pre-existing antimicrobial agents against different resistive bacterial strains. It has various properties on the basis of its functionalities such as it is non-destructive, no need for sample preparation. Moreover, it will be employed for the aqueous solutions. Raman spectroscopic analysis has been used for that of

characterization of ligands and its organometallic complexes. In present research work, Raman spectroscopy will be employed for the characterization of organometallic ligand and its Si complexes. Raman spectrophotometer with Peak Seeker Pro_785: Agiltron, USA will be used for analysis. Obtained results will be further processed via MATLAB software 7.8 (MathWorks, U.S.A). Principal components analysis (PCA) will be employed for further analyzing the organometallic ligand and its Si complexes, features of Raman spectroscopy. PCA reduces the dimensionality and increase variability between ligand from its complex.

Keywords: Raman Spectroscopy; organometallic compound; Selenium; complex and ligand; PCA.

P-44

Surface Enhance Raman Spectroscopy of RBCs for Diabetes Detection

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Abstract

Diabetes type II, also known as non-insulin-dependent diabetes, is a major health issue that affects nearly 537 million people worldwide. Different analytical techniques, such as the micro-spectrum technique, spectrophotometric analysis technique, and fluorimetry method, have been used to diagnose type 2 diabetes, but these techniques have some limitations. In current study employs surface enhance Raman spectroscopy to monitor the biochemical changes in diabetic patients' RBCs in comparison to healthy individuals. To further investigate the potential of surface enhanced Raman spectroscopy, various chemometric techniques such as PCA and PLS-DA are used. PCA distinguishes diabetic patients' RBCs from those of healthy volunteers. Furthermore, the PLS-DA method is used to distinguish and classify red blood cells (RBCs) from healthy and diabetic volunteers. The PLS-DA validation is dependent on various parameters such as receiver operating curves (ROC), accuracy, precision, and goodness of fit (R2).

Keywords: Diabetes mellitus Type 2; Red blood cells; Surface Enhance Raman Spectroscopy; PCA; PLS-DA

P-45

LIBS assisted with Machine learning Techniques

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Abstract

The purpose of the present study is the identification and classification of rock samples using Laser-Induced Breakdown Spectroscopy (LIBS) coupled with machine learning techniques. Spectra of seventeen rock samples were taken using Q-switched Nd: YAG laser operating at 532nm. The optical emission spectra were collected using Avantes spectrometer and emission spectral lines were identified using NIST atomic spectra database. To check the normality of the emission spectral data, analysis of variance (ANOVA) test was utilized which made initial differentiation. After initial discrimination, LIBS combined with principal component analysis (PCA) was applied for the complete classification of all rock samples. After improving the linearity and efficiency of PCA by support vector machine (SVM), seventeen rock samples were efficiently classified. This study demonstrated that LIBS combined with machine learning techniques (PCA, SVM) can be used for the identification and classification of the materials having large number of samples such as rocks, minerals, mines, alloys etc. This technique can be utilized for the quality check in the soil, metallurgical, and mining industries.

P-46

Synthesis and Comparative Study of Photocatalytic activity of Zinc Oxide and Zinc Ferrite nanoparticles

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Abstract

Diclofenac is an anti-inflammatory drug and a persistent water contaminant. Its presence in aqueous bodies is hazardous for both humans and the environment because it leads to the growth of harmful drug-resistant bacteria in water. The photocatalytic degradation of diclofenac under visible light irradiation was studied using Zn-Fe2O3 and simple ZnO catalysts, prepared by semi-Co-precipitation method. Both catalysts were characterized using XRD, Particle size analyzer, SEM and FTIR, and were tested for their photocatalytic activity under visible light irradiation. The photodegradation of diclofenac was investigated and the catalytic activity of prepared catalysts was observed. The reaction was observed for reaction times, the catalyst used and the presence of oxidizing agent (H2O2). Finally, maximum degradation was obtained using Zinc Ferrite nanoparticles in the absence of oxidizing agent (H2O2).

P-47

Significance of Re-Dyeability of Microwave-Assisted Sequential Stripping of Cotton Fabric Dyed with Reactive Navy

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Abstract

Color is a core element of a fabric's appeal no matter how fine its construction looks. Sometimes during the dyeing process of the textile fabrics, there occur some color variations and color spots which efficiently decrease the fabric quality. To overcome these faults, the fabric is re-dyed or the color is stripped by different mean. Though, the reactive dyes cannot be stripped efficiently from the cellulose fabric due to the establishment of the covalent bond between the fiber and dye. Some active sites of fabric remain occupied after stripping which create difficulty in redyeing process. The objective of this study was to enhance re-dyeing by fully removal of reactive navy dye from cotton using different conventional methods, with a strong attention on microwave-assisted techniques. The performance of the stripped cloth was evaluated using a spectra-flash spectrophotometer (SF-600). Microwave assisted base hydrolysis followed by reduction and oxidation gave best stripping efficiency of 98.25% for treatment time of 120 seconds each. Same treatment under conventional conditions gave 95.7% with treatment time of 30 minute each. Microwave assisted treatment revealed less damage on fabric thread in comparison with conventional one. The wrap and weft values for microwave treated sample are 9.3N and 9.2N respectively whereas 6.1N and 5.9N for conventional one. The re-dyeability of microwave treated fabric was much better than conventional method by comparing their K/S values. Hence microwave assisted technique is proved to be better in stripping efficiency, re-dyeability, minor fabric damage and time and energy saving.

P-48

Evaluation of Microwave Assisted Stripping and Re-dyeability of Cotton Fabric Dyed with Reactive Red CL4BN

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Abstract

Fabric is dyed in a range of colors but sometimes, shade attained after dyeing differs from the required shade. The problem of uneven or off-shade dyeing can be fixed by re-dyeing or by stripping of dye. Since some of the ethereal linkages between cellulose and some components of dyes like aromatic amines retained after stripping. Therefore, the active sites on the fabric are already occupied and re-dyeing is challenging. The study has been carried out to improve re-dyeing ability by totally removing the Red CL4BN dye from fabric by using sequential stripping assisted by microwave in which hydrolysis of dye-fibre bond and stripping occur simultaneously. The microwave assisted acid hydrolysis followed by reductive and oxidative stripping exhibited best stripping

efficiency of 97.11% for treatment time for 120 sec of each. The same treatment in conventional way exhibited 96% stripping efficiency for 120 sec of acid hydrolysis and 15 minutes of each reductive and oxidative stripping. Microwave stripping method resulted in less damage of the fabric as tear and tensile strength of microwaved assisted stripped fabric were larger than conventional one. The warp and weft value for microwave assisted stripped fabric was 7.3N and 7.2N respectively whereas for conventionally stripped fabric, the warp and weft values are 5.6N and 5.3N respectively. The re-dyeing ability assessed by K/S vales found to be more for microwave assisted stripping than conventionally stripped fabric. Hence microwave assisted method resulted in increased stripping efficiency, more re-dyeing ability, less fabric damage and less time and energy consumption.

P-49

Synthesis of carbon nanodots using the microwave-assisted method to investigate their catalytic and fuel additive applications

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Abstract

Carbon nanodots (CNDs) have gained much importance for their distinctive properties and promising applications. Properties of carbon nanodots such as small size, tunable fluorescence, low toxicity, high dispersibility, high photostability and low cost, make them applicable in diverse fields of modern life e.g. nanomedicine, biological and chemical sensing, catalysis, optoelectronics, bioimaging, and etc. In the present research effort, the liquid-phase synthetic approach, mainly adopting the microwave-assisted method, was utilized to synthesize carbon nanodots. Three different small organic precursors were used to synthesize carbon nanodots with different properties. Synthesized products were purified by using the membrane dialysis method. The purified products were characterized by implying different techniques e.g. XRD, Transmission Electron Microscopy (TEM), Fourier Transform Infrared Spectroscopy (FTIR) and Ultraviolet Fluorescence. XRD study showed the graphitic nature of CNDs. 3-8 nm, 13-17 nm and 4-8 nm were the average sizes, for all the three products, obtained by TEM analysis. Under UV-lamp they showed fluorescence in blue-green (turquoise) color. The catalytic potential of synthesized carbogenic nanoparticles for the degradation of Congo Red dye (CR) and as fuel additives for commercially available diesel was investigated. Under similar conditions, the rate constant for the degradation of CR dye caused by different CNDs is observed not to be equivalent. Increased CND concentrations in diesel have a considerable impact on its characteristics, indicated by the results.

P-50

A novel ofloxacin-loaded microemulsion system: Development, characterization and stability study by NMR (^{1}H & DOSY)

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Abstract

Microemulsions are transparent, isotropic and thermally stable liquid dispersion system of water, oil and stabilized by surfactants and cosurfactants. The microemulsion system is used to transport drug by virtue of the ease of preparation, high absorption rate of drug, enhanced drug solubilization, long shelf life and improved bioavailability of drug by reducing the hydrolysis of the drug. This research work was focused on enhancing the solubilization, sensitivity to various cells, and retention period of "ofloxacin" having lipophilic nature. The novel microemulsion system was formulated consisting of the olive oil (oil phase), tween 80 (surfactant), butanol (co-surfactant), and phosphate buffer (aqueous phase) loaded with 5-10% of Ofloxacin drug. The pseudo ternary phase diagram was utilized to demonstrate the internal structure of the formulated four component microemulsion system. All formulations were physically characterized by centrifugation, pH, refractive index, conductivity, surface tension and partition coefficient. The structure, purity and location of drug in the formulated microemulsion was analyzed by ^{1}H NMR analysis. The chemical shifts of the ofloxacin was determined by ^{1}H NMR. The ^{1}H NMR shows that the drug ofloxacin is located in the lipophilic region of the microemulsion. The diffusion coefficient was determined by DOSY NMR. The diffusion coefficient of the microemulsion shows that the increase in the concentration of the drug in the formulated microemulsion decrease the diffusion of the drug. Hence, it leads to conclusion that the MEs are a protective carrier due to drug entrapment ability and shield drug from hydrolysis, decomposition and oxidation. So, these are a proficient drug carrier for targeted drug delivery without toxic effect.

Keywords: microemulsion; phase behavior; ofloxacin; ^{1}H-NMR; DOSY; Stability

P-51

Optimization of RSM and Neural Network Model to predict the Behaviour of Viscosity of $NiFe_2O_4$ Based Engine oil Nanofluids

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Abstract

Heat transfer through traditional fluids such as pure water, oil, and ethylene glycol is inefficient due to their low thermal conductivity. The addition of nanoparticles to the base fluids increases the viscosity of nanofluid fluids. Changes in viscosity values can be used to investigate the rheological behavior of nanofluids. Nickel ferrite $NiFe_2O_4$ nanoparticles were made by using the sol-gel auto-combustion technique. The structure of nickel ferrite nanoparticles was determined using an X-ray diffraction (XRD) pattern. The existence of $NiFe_2O_4$ nanoparticles was confirmed in the Fourier transform infrared (FTIR) spectrum. X-ray diffraction analysis showed the single-phase face centered cubic (FCC) structure of $NiFe_2O_4$ spinel ferrite with preferred orientation along the (311) plane. The surface morphology of $NiFe_2O_4$ nanoparticles was studied using Scanning Electron Microscopy (SEM). The particle size was found 20 nm by using Scherer formula. The standard procedure was used to prepare the varied solid volume fractions of nanofluid 0, 0.25, 0.50, 0.75, and 1%. Temperatures ranging from 40-80°C were used to determine viscosity values. The viscosity of nanofluids was determined by using falling ball method.

The results of the experiment show that the viscosity of nanofluid (μ_{nf}) increases at all temperature as the volume fraction (Ø) increases. On the other hand, the viscosity of nanofluid reduces as the temperature rises. This research also proposes a new mathematically based correlation that uses the response surface approach and artificial neural networks ANNs to determine nanolubricant viscosity. The proposed mathematical correlation by response surface methodology and predicted data have R^2 values of 0.9873, which is considered good accuracy. When the performance of ANN and RSM models was compared using experimental data, it was discovered that the artificial neural network could make more accurate predictions than the RSM correlation.

P-52

In vitro Antioxidant and Antimicrobial Evaluation of various fractions of *Salvia macrosiphon* Extract

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Abstract

Plant derived medicines intrigue globally, as potential natural antioxidant and antimicrobial agents may fulfill the need of current scenarios of pandemics. The aim of current research work was to evaluate the antioxidant, antifungal and antibacterial activities of *Salvia macrosiphon* indigenous to province Baluchistan, Pakistan. Different extracts of plant stem were constituted by using methanol, butanol and water solvents through ultrasonic assisted process (UAP). Biological evaluation of extracts was done by Folin-Ciocalteu, aluminum colorimetric method, DPPH and power reducing assay to determine antioxidant potential while antimicrobial potential was determined through well diffusion method. Butanol fraction showed maximum total phenolic contents (203.80±1.96 mg gallic acid equivalent /g of DW of extract) while methanol fraction deciphered maximum total flavonoid contents (144.03±0.95 mg catechin equivalent/ g of DW of extract). Butanol fraction showed the maximum 80.00±1.00 % inhibition in DPPH assay while methanol fraction showed maximum level of 0.63±0.008 in reducing power assay. The butanol extract was found sensitive against bacterial and fungal stains such as *P. aeruginosa*, *S. aureus* and F. *brachygibbosum* as compared to all other fractions. Conclusively, butanol fraction of *salvia macrosiphon* stems was proved more effective for antioxidant, antibacterial and antifungal activities as compared to other fractions.

Keywords: Antibacterial, antioxidant, antifungal, *Salvia macrosiphon,* Ultrasonic assisted extraction technique, DPPH.

P-53

Preparation of Streptokinase Incorporated Chitosan/TPP Nanoparticles and their in vitro analysis

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Abstract

To overcome cardiovascular diseases thrombolytic agents are widely used. Among them one most preferable is streptokinase (SK) because of its efficiency and low-cost production but its immunogenic nature sometimes causes severe complications. To make it more effective drug various techniques have been introduced. Nanotechnology is emerging in thrombolytic therapy as one such technique to make thrombolytic more effective. In this research, Chitosan polymer nanoparticles were used to entrap streptokinase (SK) and to check its thrombolytic potency after incorporation. Streptokinase purified from streptococcus pyogenes EBL-45 was used for entrapment purpose. Nanoparticles with size ranging in 193.4-392 nm were obtained when protein concentration was 0.1-0.5 mg/mL respectively. On the other hand, zeta potential decreased upon increasing protein concentration i.e., from 15.3 mV to -13 mV. Encapsulation efficiency was increased on increasing protein concentration to certain limit i.e., 0.3 mg/mL and then started to decrease. SEM results showed that nanoparticles were of uniform size with slightly aggregation. FTIR spectra of prepared nanoparticles confirmed cross-linking between chitosan and TPP. It also presented characteristic peaks of streptokinase which predicts that SK

maintained its functionality after incorporation. Activity of SK was determined by radial caseinolysis and blood clot lysis and by both methods it was confirmed that SK activity reduced non-significantly after incorporation.

Keywords: streptokinase, chitosan, nanoparticles, SEM, FTIR

P-54

Neuroprotective effect of Perampanel on pilocarpine induced status epilepticus in mice

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Abstract

Status epilepticus was defined as a continuous seizure for 5min, recurrent seizures activity without recovery, and continuous electrographic or clinical seizure. Features of SE include injury in the limbic region, epileptic foci development, later on, the process of epileptogenesis started which led to SRS development. Pilocarpine-induced SRS are produced by acting on glutamatergic receptors, causing cell death by contributing to seizure sustenance. Behavioral alterations and impaired memory and learning are also observed in patients with SE. This study aimed to explore the anti-seizure potential of Perampanel an α-amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid (AMPA) receptor antagonist in pilocarpine-induced acute status epilepticus in mice. Pilocarpine was used to induce status epilepticus in adult BalbC mice. Perampanel was administered after 30minits of SE onset. By electroencephalogram recordings efficacy of different doses of Perampanel (2, 4, 6 and 8mg/kg) was assessed. In addition, behavioral score of motor seizure was also recorded. Our results indicate that post-treatment with perampanel significantly reduced seizure activity. Moreover, perampanel treatment led to reduce frequency and amplitude of seizures in dose-dependent manners. Our study reveals that SE induced long term consequences can be modified by blocking AMPA receptors by perampanel. To our knowledge this is first of its kind activity that has never been performed earlier on mice.