

CURRICULUM VITAE

1. PERSONAL DATA

Name: Prof. Dr. Sumera Zaib

Place of Birth: Mansehra

Nationality: Pakistani

Contact Address: Department of Basic and Applied Chemistry, Faculty of Science and Technology, University of Central Punjab, Lahore 54590, Pakistan.

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2. ACADEMIC/PROFESSIONAL PARTICULARS

(a) Field of Specialization:

Biochemistry, Clinical Biochemistry, Enzymology, Protein expression, Drug Designing & Bioinformatics.

(b) Academic Qualifications

- Doctor of Philosophy, Biochemistry, 2016, Hazara University, Mansehra, Pakistan, Biological Evaluation of Novel Ionic Liquids and Coordination Complexes, 4.00
- Master of Philosophy, Biochemistry, 2010, Hazara University, Mansehra, Pakistan, Toxicity and effects of methanolic extract and fractions of Cedrela serrata against Tribolium castaneum (Coleoptera: Tenebrionidae), 4.00
- B.Sc (Hons), Biochemistry, 2007, Hazara University, Mansehra, Pakistan, Evaluation of Heavy Metals in Soil, Water and Vegetables using Flame Atomic Absorption Spectroscopy (FAAS), 3.92
- Diploma in Homeopathic Medical Science (D.H.M.S) (R.H.M.P), 2004-2008, Homeopathic Medical College, Mansehra, Pakistan, 75%
- Higher Secondary School Certificate (Pre-medical), 2001, Board of Intermediate & Secondary Education, Abbottabad, Pakistan
- Secondary School Certificate (Science group), 1999, Board of Intermediate & Secondary Education, Abbottabad, Pakistan

(c) Academic Honors and Awards

- UCP Best Researcher and Innovator Award from UCP for 2021.
- HEC Indigenous Scholarship for Ph.D studies (2012-16).
- DAAD Summer School Visit to Bonn, Germany, 2014.
- DAAD study visit to Germany in 2014.
- Research Productivity Award 2017-2018 by Pakistan Council for Science and Technology (PCST), Islamabad in category D.
- Research Productivity Award 2012, 2013, 2014, 2015, 2016, 2017 &

2019 by COMSATS University, Islamabad.

- 2nd position in BSc (Hons.) & 1st position in M.Phil.
- Shaheen fellow in each year of M.Phil studies.

(d) Membership of Professional Bodies

(e) Language Proficiency

English (Spoken and written)-C1

Urdu (Spoken and written)-C2

3. CAREER DETAILS

(a) Academic Positions Held

- Professor at Department of Basic and Applied Chemistry, Faculty of Science and Technology, University of Central Punjab, Lahore from 1st January 2025 to date.
- Associate Professor at Department of Biochemistry, Faculty of Life Sciences, University of Central Punjab, Lahore from November 2021 to December 2024.
- Assistant Professor at Department of Biochemistry, Faculty of Life Sciences, University of Central Punjab, Lahore from August 2019 to October 2021.
- Post-doctoral Research Associate from September 2018 to July 2019 at COMSATS University Islamabad, Abbottabad Campus.
- Assistant Professor at International Islamic University, Islamabad from August 2017 to August 2018.
- Post-doctoral Research Fellow at COMSATS University Islamabad, Abbottabad Campus from May 2015 to August 2017.
- Research Scholar at COMSATS University Islamabad, Abbottabad Campus from November 2010 to April 2015.
- Demonstrator at Abbottabad International Medical College, Abbottabad, from April 2007 – April 2008.
- Lecturer at Abbottabad International Medical College, Abbottabad, from July 2011 – December 2012.
- Internee under National Internship Program at Hazara University, Mansehra, Pakistan from July 2010 – June 2011.
- Internship experience from Ayub Teaching Hospital, Abbottabad as an internee in Hematology lab, Blood bank, Microbiology lab and Chemical pathology lab.

(b) Administrative Positions Held

- Head of Department, Department of Biochemistry, Faculty of Science and Technology, University of Central Punjab Lahore from June 2022 to June 2025.

4. Teaching

(a) Summary of Courses Taught

Course Code, Course Name, credit hours

- BIOCHE2013, Biochemistry (Credit Hr=2+1)
- BT 625 Principles of Biochemical Engineering (Credit Hr=3)
- BT 521, Protein Engineering (Credit Hr=3)

- BIOCHE1123, Advanced Techniques in Biochemistry (Credit Hr=3)
- BIOCHE5033, Clinical Biochemistry (Credit Hr=2+1)
- HUMPHY1023, Human Physiology (Credit Hr=3)
- BC5273, Advanced Clinical Biochemistry
- CTISSU7013, Cell and Tissue Culture
- BC682, Advances in Endocrinology
- BC725, Human Genetics
- CH615, Medicinal Chemistry
- BC683, Recent Trends in Immunology
- BI 654, Computational Biology
- BI 728, Methods in Bioinformatics
- BI 611, Computational Drug Designing

(b) Participation in Academic Accreditation

Member of National Curriculum Review Committee (NCRC)

Nominated by HEC as for BS and MS Chemistry (14th -15th November, 2024)

Development Curriculum Review Committee Chair, (2022 onwards) & member (2019 to onwards)

Industrial Advisory Board Chair, (2022 onwards) & member (2019 onwards)

Board of Studies, Chair, (2022-2025) & member (2019 onwards)

Board of Faculty, Head of Department, (2022-2025) & member (2019 onwards)

Academic Council Meeting, Member, (2021 onwards)

Board of Advanced Studies, Member, (2021 onwards)

Ethical Review Board, Committee member, (2021 onwards)

(c) Research Students Supervised/Trained

<u>Level</u>	<u>Number of Trainees</u>
PhD Students	15
Master Students	>41
Undergraduate Students	>85

PhD

<u>Sr No</u>	<u>Names</u>	<u>Titles</u>	<u>Status</u>	<u>Year of Completion</u>
1	Aisha Nawaz	Isolation and characterization of bioactive compounds from <i>Silybum marianum</i> and their antiproliferative potential	Completed	2022
2	Shabbir Ahmad	Association of Inflammatory Markers Among Patients with Diabetes Mellitus and Peripheral Arterial Disease	Completed	2023

3	Mohaamad Tayyab Yunus	Exploring the Structural Diversity of Synthetic Compounds to Evaluate Their Potential Against Neurodegenerative Disorders	Completed	2023
4	Shabab Zahra	Discovery and Development of New Heterocyclic Drug Candidates for Diabetic Complications	Completed	2024
5	Ahmad Hassan	Molecular mechanisms of plant-derived inhibitors involved in the management of <i>Fusarium oxysporum</i>	Completed	2024
6	Asma Arshad	Effectiveness of using Variable Number Tandem Repeat (VNTR) to rule out Maternal Cell Contamination in Prenatal Diagnosis for β -thalassemia	Completed	2024
7	Lateef Ullah	Design, synthesis, in vitro and in vivo evaluation of inhibitors of lipoxygenase, cyclooxygenase 1 and cyclooxygenase 2 to mitigate chronic inflammation	Research in progress	-
8	Nehal Rana	Harnessing the Untapped Therapeutic Potential of Phthalazine scaffold as Small-molecule Inhibitors of Ectonucleotidases for the Treatment of Diabetic Complications	Research in progress	-
9	Anwar Khalid	Synthesis, Characterization, and Evaluation of Immunomodulating Anticancer Compounds using 3D Tumor Model	Research in progress	-
10	Sundus Waheed	Efficacy of Lacticbacillus species probiotic strain to treat nickel induced dermatitis	Synopsis Writeup	-
11	Faryal Toqueer	-	Course work	-

MS students

<u>Sr No</u>	<u>Names</u>	<u>Titles</u>	<u>Status</u>	<u>Year of Completion</u>
1.	Qurat-ul-Ain	Antileishmainial activity of metallic complexes	Completed	2019
2.	Urooj Yousaf Virk	Antiproliferative and proapoptotic effect of Daucus carota in cervical cancer cells: <i>In-vitro</i> approach	Completed	2021
3.	Zainab Tajammul	Virtual screening, design and synthesis of phthalazine derivatives as cholinesterase inhibitor: Evaluation of biochemical studies	Completed	2021
4.	Marriyam Ramay	Design and synthesis of metal-based urease inhibitors: <i>In-Vitro</i> and <i>In-Silico</i> analysis	Completed	2021
5.	Hafiza Hafsa Tahir	Formulation and optimization of metal-based nanoparticles of <i>Withania somnifera</i> aqueous fruit extract for cancer therapy by <i>in-vitro</i> and <i>in-silico</i> analysis	Completed	2021
6.	Sabir Khan	Extraction, Purification and Characterization of	Completed	2021

		trypsin inhibitor protein from soyabean seeds		
7.	Bakhtawar Bukhari	Green synthesis of silver nanoparticles using <i>Acer oblongifolium</i> and its antibacterial effect and antiproliferative activity against human cancer cell lines (MCF-7, HeLa)	Completed	2021
8.	Hafiza Taha Maryam	Harnessing the Untapped Therapeutic Potential of Sulfonamide Derivatives: Accessing Small-Molecule Inhibitors of Carbonic Anhydrases	Completed	2022
9.	Hamza Asghar	Phytochemical characterization of <i>Prunus persica</i> leaves & their biological activities	Completed	2022
10.	Kiran Shahzadi	<i>In-Vitro</i> and <i>In-Silico</i> Evaluation of Inhibitory Potency of Sulfonate and Sulfamate Derivatives Against Carbonic Anhydrases	Completed	2022
11.	Muhamad Zain Altaf	<i>In-Vitro</i> and <i>In-Silico</i> Analysis of Benzenesulphonamide Derivatives against alpha-Glucosidase for Treatment of Diabetes	Completed	2022
12.	Syed Talha Liaqat	Mutational Analysis of Duchenne Muscular Dystrophy and <i>In-Silico</i> Approaches for its Therapeutics	Completed	2022
13.	Huma Riaz	Monoamine Oxidase Inhibition Activity of Synthesized Acetophenone and Thiophene Substituted Hydrazide Derivatives: <i>In-Vitro</i> and <i>In-Silico</i> Bioevaluation	Completed	2022
14.	Mujeeb Ur Rehman	Drug Designing and Screening of Alkaline Phosphatase Inhibitors	Completed	2022
15.	Fatima Akram	Genetic Polymorphism in Methylenetetrahydrofolate Reductase Gene Associated With Epilepsy And <i>In-Silico</i> Rational Design For Its Therapeutics	Completed	2022
16.	Ayesha Akram	Identification and association of MIF-173 G/C Polymorphism Gene with the Risk of Acute Myeloid Leukemia and Mutational Analysis of the Gene	Completed	2023
17.	Laryib Shahid	Role of DPP-4 inhibitors in the treatment of Type 2 Diabetes Mellitus	Completed	2023
18.	Tahira Aslam	Phytochemical characterization and biological activities of <i>Punica granatum</i> peel	Completed	2023
19.	Noshaba Mehmood	Enzymes-mediated mycotoxins degradation by non-toxic fungi in cereal crops	Completed	2023
20.	Nehal Rana	Discovery of Benzyl Carboxamide Derivatives as Potent Inhibitors of Beta-Secretase for the Management of Alzheimer's Disease	Completed	2023
21.	Areeba	Evaluating the inhibitory activity of Aldo reductase enzyme against bioactive compounds	Completed	2023
22.	Hira Javed	Investigation of inhibitory potential of pyrimidine-morpholine hybrid compounds against Angiotensin Converting Enzyme	Completed	2023
23.	Toaqeer Salman	Oxygen evolution by using Photoanodic Ta ₃ N ₅ for water splitting process by different surface modifications	Completed	2023

24.	Aqsa Hayyat	Comparative biochemical and nutritional assessment of basil, chia, and flax seeds against chemical-induced hyperlipidemia	Completed	2023
25.	Noor Ul Huda	Association of Phospholipase A2 Receptor 1 (PLA2R1) rs35771982 Gene Polymorphism with Idiopathic Membranous Nephropathy in Population of Lahore	Completed	2023
26.	Raheel Waseem	Identification of Colistin Resistance Mcr-8 and Mcr-10 Genes in Clinical strains of Escherchia coli, Pseudomonas aeruginosa and Klebsiella pneumoniae from Lahore Pakistan	Completed	2023
27.	Aneeza Asghar	Discovery of derivatives as potent inhibitors of glutathione peroxidase for the management of cancer disease	Completed	2024
28.	Afifa Tur Rehman	Extraction, purification, characterization and invitro analysis of synthetic derivatives against lipoxygenases	Completed	2024
29.	Usman Wajid	Clinical significance of serum prostate specific antigen in prostate cancer patients and its relationship with hypercholestrolemia	Completed	2024
30.	Ayesha Zahid	Chemical and biological Effects of Coloring agents in Soft Drinks on Human Health	Completed	2024
31.	Ravish Fatima	Optimizing Recombinant Expression of Human Growth Hormone in <i>E. coli</i> for Cost-Efficient Production	Completed	2024
32.	Kainat Ahsan	Identification and Screening of Dual Inhibitors of Monoamine Oxidase B and Angiotensin Converting Enzyme	Completed	2024
33.	Dur e Kashaf Jaffery	Drug design,synthesis and characterisation of dual inhibitors against urease and carboic anhydrase	Completed	2024
34.	Amna Eman	Synthesis and Characterization of Specific Inhibitors of Cholinesterases against Alzheimer's disease: <i>In Vitro</i> and <i>In Silico</i> Analyses	Completed	2024
35.	Romaisa Irfan	Revolutionary approach to produce bioactive human parathyroid hormone using <i>E. coli</i> as expression host	Completed	2025
36.	Faraz Nabeel Taj	Synthesis, Characterization, and Biological Activities of Inhibitors Against Glucosidases and Amylase	Completed	2025
37.	Sherian khattak	Extraction, isolation and purification of cyclooxygenase-2 and identification of its selective inhibitors	Completed	2025
38.	Iman Rehman	Synthesis, characterization and evaluation of dual metal nano zerovalent particles incorporated on date palm biochar for the remediation of antibiotics from pharmaceutical wastewater	Thesis Write up	2025
39.	Eman Fatima	Targeting Triple Negative Breast Cancer Using Drug Repurposing	Thesis Write up	2025

40.	Summayya Maryam	Extraction, Purification of cyclooxygenase-1 and screening of inhibitors.	Thesis Write up	2025
41.	Qasia Saba	Development of an ecofriendly formulation using Omega-3 Fatty acids and Fat-Soluble Vitamins for primary health benefits	Research in progress	-
42.	Noor Fatima	A Novel Approach for the Extraction and Isolation of Ecto-Nucleoside Triphosphate Diphosphohydrolase 3	Research in progress	-
43.	Anmol Fatima	Green Synthesis of Silver Nanoparticles from Telfairia occidentalis for Enhancing Soil Fertility and Plant Growth	Research in progress	-
44.	Areej Fatima	Enhanced Self-Healing, Robust Mycelium Leather from Ganoderma lucidum for Sustainable Applications	Research in progress	-

(d) Participation in Thesis and Oral Examination Committees

<u>Level</u>	<u>Number of Examinations</u>
PhD Students	20
Master Students	>150

(e) Training

- United Nations Office on Drugs and Crime (UNODC) Integrity, Ethics, and Anti-Corruption Module – Cohort 4, Punjab University Pharmacy College and Ramada Lahore, Pakistan, Period 01/2025-02/2025.
- Intellectual Property, University of Central Punjab, Pakistan, Period 08/2023-09/2023.
- Program Assessment Process, University of Central Punjab, Pakistan, Period 08/2023-09/2023.
- Balanced Scorecard Bootcamp, by First Promethean, Management Research & Services, University of Central Punjab, Pakistan, Period 11/2023-11/2023.
- Research Capacity Building Programme for Researchers, Pak-UK Education Gateway by British Council, Pakistan, Period 2022.
- BASIC FIRST AID TRAINING, University of Central Punjab, Pakistan, Period 08/2022-08/2022.
- Developing Industrial Linkages, Pakistan, Period 08/2022-08/2022.
- Teaching Excellence Program conducted by University of Central Punjab, Pakistan, Period 09/2021-09/2021.
- Faculty Development Program, University of Central Punjab, Pakistan, Period 09/2020-09/2020.
- Practical Training Session on Publication Writing and Citation Management using Endnote, University of Central Punjab, Pakistan, Period 10/2019-10/2019.
- Faculty Development Program, University of Central Punjab, Pakistan, Period 09/2019-09/2019.
- Research paper, data analysis and thesis writing, Hazara University, Mansehra, Period 06/2013-06/2013.

(f) e-learning Course Taught

Clinical Biochemistry, ARVO-Traditional Education in a Digital Way, (2024-onwards)

5. RESEARCH

(a) Research Interests

- Clinical Biochemistry especially, Thalassemia, Diabetes, Acute Myeloid Leukemia, Cystinuria, Alzheimer's disease & Parkinson's disease, Idiopathic Membranous Nephropathy
- Enzyme inhibition and extraction
- Protein expression
- Histopathology of liver, brain, pancreas, kidneys,
- Osteochondral regeneration
- Drug designing and delivery
- Medicinal chemistry
- Nano composite preparation and encapsulation
- Organic synthesis
- Mutational analysis
- Biomarker identification
- Vaccine designing
- Bioinformatics and computational biology
- Structural biology and molecular biology
- Toxicological evaluation of natural and synthetic compounds
- Nutraceutical product development
- Genetic engineering

(b) Publications/Citations Data

<u>Type of Publication</u>	<u>Number of Publications</u>
Articles in International Refereed Journals	<u>202</u>
Books/Book Chapters	<u>Books: 1; Book Chapters: 7</u>
Patents	<u>9 (National Patents)</u>
 <u>Citation Source</u>	 <u>Number of Citations</u>
<u>Google scholar</u>	<u>4950</u>

(c) Research Grants

- Research project, Principle Investigator, Harnessing the Untapped Therapeutic Potential of Phthalazine scaffold as Small-molecule Inhibitors of Ectonucleotidases for the Treatment of Diabetic Complications, Pakistan Science Foundation, 12/2023-present, 4.65 Million (in Process).

- Scientific Challenge, Principle Investigator, *Development of Novel Selective Inhibitors of HIPK3 by In silico Lego-like Approach to Treat Huntington's Disease*, BioSolveIT, 2023, 5000 Euros (Completed).
- Scientific Challenge, Principle Investigator, *Serine Protease Enzymes for the Discovery of Novel Inhibitors to Combat COVID-19*, BioSolveIT, 2020-2021, 1.793 Millions (Completed).
- Research Project, Principle Investigator, *Mechanism of apoptosis in Leishmania tropica promastigotes induced by Pentavalent Antimonials*, Higher Education Commission, 6 months, 0.5 Millions (completed).

(d) Patents

1. Synthesis of Leather from Genetically Modified Mushroom, Sumera Zaib, 2023, University of Central Punjab
2. Development of Need Based Smart Hands for Mute to convert Sign-language to Voice, Sumera Zaib, 2023, University of Central Punjab
3. Discovery of lead inhibitor against mutant TET2 to treat acute myeloid leukemia, Sumera Zaib, 2023, University of Central Punjab
4. Evaluation of Anticancer Potential of Hybrid Chitosan-Silver Nanoparticles Containing Aqueous Fenugreek Seed Extract; In Vitro and In Vivo Studies, 2022, Sumera Zaib, University of Central Punjab
5. Synthesis and Characterization of Hybrid Chitosan-Silver Nanoparticles Containing Aqueous Fenugreek Seed Extract, Sumera Zaib, 2022, University of Central Punjab
6. In Silico Vaccine Design for Parasitic Entamoeba histolytica Based on SHERP multiepitopes, Sumera Zaib, 2022, University of Central Punjab
7. Development of novel combination therapy for estrogen receptor-negative breast cancer, Sumera Zaib, 2022, University of Central Punjab
8. Finding fibroblast growth factor receptor 3 lead inhibitor to treat achondroplasia, Sumera Zaib, 2022, University of Central Punjab
9. Exploration of the specific inhibitors of yellow fever helicase and NS5 protein to treat yellow fever virus infection, Sumera Zaib, 2022, University of Central Punjab

(e) Participation in Regional & International Conferences

- Virtual Symposium on "Frontiers of Vaccine Design and Immunology: Unveiling the Latest Advances" by Faculty of Science and Technology, University of Central Punjab on 25th September, 2023.
- 7th International Symposium on "Environmental health and Biosecurity Strategy" by Obuda University on 4-5th May, 2023.
- 6 sessions (2 hours per session) Workshop on "Intellectual Property" from 23rd August to 27th September, 2023.
- The International Conference on Food and Applied Sciences (ICFAS-2023) Dir-Kumrat at Shaheed Benazir Bhutto University Sheringal, (Dir) KPK held in August 2023.
- Faculty Industry Placement Program (FIPP) from 28th August, 2023 to 1st September, 2023 at NovaMed Pharmaceuticals.
- Training workshop on "Program Assessment Process" conducted on 12th September, 2023.

- "Biosymposium: Structural Biology Approaches in Drug Discovery and Vaccine Research" conference and hands-on-workshop organized by Department of Biology, Lahore University of Management and Sciences on March 13th-14th, 2023.
- One Day Seminar on "Cervical Cancer Awareness" held on 10th January, 2023 and organized by Department of Microbiology, Faculty of Science and Technology, University of Central Punjab, Lahore.
- Successfully completed "Balanced Scorecard Bootcamp" by First Promethean, Management Research & Services on 23rd-24th November 2023.
- Completed four-day training course on "Research Capacity Building Programme for Researchers" conducted under Pak-UK Education Gateway by British Council in 2022.
- Two days training of "BASIC FIRST AID TRAINING" during August 30th - 31st 2022 at University of Central Punjab.
- Attended one-day workshop on "Developing Industrial Linkages" conducted on 5th August 2022.
- Actively participated in 8th Asia Pacific Probiotics Symposium held on 6th December 2021.
- Teaching Excellence Program conducted by University of Central Punjab during September 6th – 9th 2021.
- Two Days Training "Faculty Development Program" during September 8th – 9th 2020 at University of Central Punjab, Lahore.
- Bioinformatics Model Competition and presentation on 5th February, 2020 at University of Central Punjab, Lahore.
- "Practical Training Session on Publication Writing and Citation Management using Endnote" on 9th October, 2019 at University of Central Punjab, Lahore.
- One Day Workshop on "Bioassay for Bioactive Compounds Isolates from Medicinal Plants" on 3rd October, 2019 at University of Central Punjab, Lahore.
- One Day Symposium regarding "Biochemical Techniques used in Diagnostics Labs" on 20th September, 2019 at University of Central Punjab, Lahore.
- Two Days Training "Faculty Development Program" during September 17th – 18th 2019 at University of Central Punjab, Lahore.
- One Day Seminar on "Bio waste Management Training" was arranged with collaboration of FLS and Pakistan Biological Safety Association on 5th September, 2019 at University of Central Punjab, Lahore.
- 3rd INTERNATIONAL CONFERENCE ON RECENT INNOVATIONS IN PHARMACEUTICAL (ICRIPS) on March 13th -14th 2019 in Islamabad.
- Oral presentation in 1st International Conference on "Advancements in Biotechnology & Biocomputing" organized by Department of Biological Sciences, International Islamic University, Islamabad during 7-9 February, 2019.
- Oral presentation in two-day National conference on "*Recent Advancements in Pharmaceutical Sciences: Innovative Drug Research for Better Cure*" during 7-8 March, 2018, organized by College of Pharmacy, University of Sargodha, Pakistan.
- Poster presentation in International Conference on Chemical and Pharmaceutical Sciences: Recent Approaches in Research & Applications, during 17-19 January, 2018 at Forman Christian College (A Chartered University) Lahore, Pakistan.

- Oral presentation in 1st International Conference on Advances in Drug Discovery and Development" during 3-5 January, 2018 at NARC, Islamabad, Pakistan.
- Workshop on Drug Design and Discovery in 2nd International Conference on Recent Innovations in Pharmaceutical Sciences (ICRIPS-2017), November 15-16, 2017, Riphah International University, Islamabad, Pakistan
- Active Participant in 2nd International Conference on Recent Innovations in Pharmaceutical Sciences (ICRIPS-2017), November 15-16, 2017, Riphah International University, Islamabad, Pakistan.
- Hands-On Workshop on Flow cytometry: Principles, Applications and Data Analyses held on 25-26 October, 2017 at Alpha Genomics Private Limited, Islamabad.
- Active participant in Conference on "Computational Biology and Genomics" (September 27-29, 2017) organized by the Center for Human Genetics, Hazara University, Mansehra.
- Active participant in workshop on "Bioinformatics and Computational Drug Designing" (January 27-28, 2017) organized by Kinnaird College for Women, Lahore.
- Active participant in 1st Biennial Conference on "New Horizons in Drug Discovery and Pharmaceutical Science" (December 15, 2016) organized by Abbottabad University of Science and Technology, Abbottabad.
- Active participant in National Conference on "Recent Innovations in Pharmaceutical Sciences" (October 25-26, 2016) organized by Riphah International University, Islamabad.
- Oral presentation in 13th Biennial Conference on "Recent Advances & Challenges in Molecular Biology, Biochemistry and Biotechnology" (25-27 August, 2016) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- Active participant in "2nd International Conference on Drug Development-Natural & Synthetic" (August 23-25, 2015) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- Poster presentation at International Conference on "Exploring New Avenues In Medicinal Chemistry: Opportunities And Challenges" (January 21-23, 2015) organized by Department of Chemistry, Forman Christian College (A Chartered University) Lahore.
- Active participant in "Three days Workshop on DNA Sequencing" (February 10-12, 2014) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- Active participant in Three-Day workshop on Computational Chemistry (January 7-9, 2014) organized by Department of Chemistry, Forman Christian College (A Chartered University) Lahore.
- Active participant in "International Symposium on Drug Development- Natural & Synthetic" (August 25-27, 2013) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- One day training workshop on "Research paper, data analysis and thesis writing" (June 14, 2013) organized by the Department of Biochemistry, Hazara University, Mansehra.

- Active participant in One Day Symposium on "Applied Aspects of Health Sciences" (May 21, 2013) organized by the Department of Biochemistry, Hazara University, Mansehra.
- Oral presentation in 31st Pakistan Congress of Zoology (International) held at University of Azad Jammu & Kashmir, Muzaffarabad (April 19-21, 2011).
- Active participant in 9th international and 21st national Chemistry Conference jointly organized by the Department of Chemistry and International Center for Chemical and Biological Sciences (March 14-16, 2011) held at HEJ Karachi.
- Oral presentation in 30th Pakistan Congress of Zoology (International) held at University of Agriculture, Faisalabad (March 2-4, 2010).
- Oral presentation in International Science Conference on "Utilization of Modern Agriculture Technology in Changing Environmental Perspectives" (July 21-23, 2010) held at Faculty of Agriculture, Rawalakot, The University of Azad Jammu & Kashmir.
- Active participant in Three-Day International Symposium on Basic Techniques in Research, Dissertation and Paper Writing in Life Sciences (July 27-29, 2010) conducted by Department of Zoology Hazara University, Garden Campus Mansehra.
- Active participant in One day National Seminar on "Enhancement of natural beauty through conservation of animals and birds" (June 4, 2009) organized by Department of Zoology Hazara University, Garden Campus Mansehra.

6. SERVICE

(a) Member of National Curriculum Review Committee (NCRC)

Nominated by HEC as for BS and MS Chemistry (14th -15th November, 2024)

(b) Scientific Societies Membership

Associate Secretary of Pakistan Society for Biochemistry and Molecular Biology (PSBMB) from June 2024 to date.

(c) Membership of Institutional, National, or International Scientific Advisory Boards

University of Central Punjab/Board of Advanced Studies and Research (BASR), Committee member, 2022-present.

(d) Membership of Conference Committees

Organizing Committee,
Registration Committee,
Accommodation Committee,
Finance Committee,

At 7 different national and International Conferences at COMSATS University Islamabad (Abbottabad Campus) and University of Central Punjab, Lahore during 2013 to 2022.

(e) Service as Reviewer

Journals

- Bioorganic & Medicinal Chemistry Letters, ISSN No. 0960-894X, Elsevier
- Bioorganic Chemistry, ISSN No. 0045-2068, Science Direct
- Pharmaceutical Research, ISSN No. 0724-8741, Springer
- European Journal of Medicinal Chemistry, ISSN No. 0009-4374, Elsevier
- MedChemComm, ISSN No. 2040-2503, Royal Society of Chemistry
- RSC Advances, ISSN No. 2046-2069, Royal Society of Chemistry
- Bioorganic & Medicinal Chemistry, ISSN No. 1464-3391, Elsevier
- Medicinal Chemistry, ISSN No. 1554-8120, Bentham Science
- Nutrition Review, ISSN No. 0029-6643, Oxford University Press
- Journal of Molecular Structure, ISSN No. 0022-2860, Elsevier
- Arabian Journal of Chemistry, ISSN No. 1878-5352, King Saud University
- Applied Organometallic Chemistry, ISSN No. 1099-0739, Wiley
- Current Topics in Medicinal Chemistry, ISSN No. 1568-0266, Bentham Science Publishers
- MDPI Journals

Conferences

- ICAI (International Conference on Artificial Intelligence), Jinnah Auditorium (Islamabad, Pakistan), 2023
- ICAI (International Conference on Artificial Intelligence), Jinnah Auditorium (Islamabad, Pakistan), 2022

(f) Membership of Journal Editorial Boards

- Designing Next-Generation Drug-Like Molecules for Medicinal Applications for International Journal Molecules, ISSN No. 1424-8247, MDPI (since: 07/2020)
- Frontiers in Pharmacology and Frontiers in Oncology, ISSN No. 2234-943X, Frontiers (since: 08/2020)
- Frontiers in Protein Chemistry and Enzymology, ISSN No. 2296-2646, Frontiers (since: 08/2020)
- Frontiers in Pharmacology, ISSN No. 1663-9812, Frontiers (since: 08/2020)
- Frontiers in Molecular Biosciences, ISSN No. 2296889X, Frontiers (since: 08/2020)
- Frontiers in Chemistry, ISSN No. 2296-2646, Frontiers (since: 08/2020)

(g) Invited Presentations at Scientific Meetings/Workshops

- Expert Lecture on "Good Laboratory Practices (GLP)" at National Centre of Industrial Biotechnology (NCIB), Pir Mehr Ali Shah Arid Agriculture University, Rawalpindi on 5th March, 2025.
- Invited talk on "Synergizing AI, CADD, and Nanoinformatics: Accelerating Drug Development for Complex Diseases." at Department of Chemistry at the University of Haripur on 6th March, 2025.
- Invited talk on "Translating Bioinformatics Research into Clinical Practice: Opportunities and Hurdles" at a seminar at the International Islamic University, Islamabad on December 6, 2024.
- Advancing Frontiers in Allied Health Research: Innovations, Impact, & Methodologies 2024" organized by Faculty of Allied Health Sciences at Gomal

University, DI Khan on 17th October, 2024.

- "Pakistan Paints & Construction Chemicals-2024" held on 19th-21st September, 2024 at Lahore Expo Center organized by Pakistan Coating Association.
- Invited Speaker at "Pakistan Chemical Forum" at International Expo Center, Lahore on 6th March, 2024 organized by Pakistan Chemical Council.
- Invited Speaker at "International Conference on Research Advancements in Chemistry-2024" on 21st-23rd August, 2024 organized by National University of Science and Technology, Islamabad.
- Invited Speaker at "Pakistan Chemical Forum" at International Expo Center, Lahore on 6th March, 2024 organized by Pakistan Chemical Council.
- Harnessing the untapped therapeutic potential of small-molecule inhibitors in pharmaceutical industry, 10th Emirati-German Congress in Medicine, Dental Medicine & Pharmacy organized by Colleges of Medicine and Health Sciences, University of Sharjah (Sharjah, Dubai), 5-6th February, 2024.
- Identification of isobenzofuranone derivatives as promising antidiabetic agents: Assessment of enzyme inhibition studies and computational docking analysis, International Conference on Life Sciences: Exploring the Frontiers in Biological Sciences organized by University of Management Sciences (Lahore, Pakistan), 13th December, 2023.
- 1st International Conference on New Horizons in Medical Sciences organized by Gomal Medical College (Dera Ismail Khan, Pakistan) 3rd-4th, February 2023.
- Discovery and Development of Heterocyclic Drug Candidates for Diabetic Complications, International Conference on Research Advancement in Chemistry (ICRA-C) organized by Department of Chemistry, SNS-NUST (Islamabad, Pakistan) August 24th – 25th 2022.
- 19th International and 31st National Conference on "Emerging Trends in Chemistry" at University of Management and Technology (Lahore, Pakistan) December 16-18th 2021.

(h) Jury Member in Conferences

- PSBMB 15th Biennial International Conference "Trends in Molecular Biology" at Punjab University, Lahore from 14th-17th April, 2025
- Chief moderated in the *2nd International Conference on Emerging Horizons in Science and Technology (ICEHST)-2024* conference held at University of Central Punjab from Nov 21-22, 2024.
- Jury Member in Poster, painting and model competition held on World Food Day, 2024 organized by Department of Food Science and Technology, UCP on October 23, 2024.
- Acted as Judge at *International Conference on Research Advancements in Chemistry-2024* on 21st-23rd August, 2024 organized by National University of Science and Technology, Islamabad.
- Acted as Jury member for *2nd Food Innovation Competition & Expo 2024*, organized by Department of Food Science and Technology, Faculty of Science and Technology, University of Central Punjab.
- Acted as Jury Member in "*8th Molecular Models & Bioinformatics Poster Competition A Gateway to Entrepreneurship*" held on 1st February 2024 organized by Department of Biotechnology, Faculty of Science and Technology, University of Central Punjab.
- Actively participated as Jury Member in "*Food Innovation Competition 2023*" organized by Department of Food Science and Technology, FOST and Food Junction Society, University of Central Punjab, Lahore, Pakistan, held on February 07, 2023.

- Participated as a Judge at International Conference on Research Advancement in Chemistry (ICRA-C) on August 24th – 25th 2022 organized by Department of Chemistry, SNS-NUST, Islamabad.

(i) Conferences/Seminars/Trainings Organized

- 15th Biennial International Conference "Trends in Molecular Biology" at Punjab University, Lahore from 14th-17th April, 2025.
- NAPRECA Winter School 2024 on medicinal plant production "Socio-Economic Importance of Medicinal Plant Production" at University of Central Punjab, Lahore from Nov 25–28, 2024.
- "6th One-Day Lab Introductory Hands-on-Training/workshop of Department of Basic and Applied Chemistry on 3rd October, 2024.
- One Day International Webinar on Nuclear Magnetic Resonance (NMR): From Fundamentals to Applications on 28th December, 2023.
- "5th 1-Day Lab Orientation & Hands-on-Training/workshop of Department of Basic and Applied Chemistry on 1st August, 2023.
- Chief organizer of the dermatology session healthcares medical consultation in collaboration with University of Central Punjab in July, 2023.
- "4th 1-Day Lab Orientation & Hands-on-Training/workshop for Biochemistry Research Students" conducted by Department of Basic & Applied Chemistry on 22nd March, 2023.
- "UCP Science and Engineering FEST-2023" organized by the Faculty of Engineering and Faculty of Science and Technology, University of Central Punjab, Lahore on 7th -8th March, 2023.
- "1st National Conference on Emerging Horizons in Science & Technology" held on December 26-27, 2022 in University of Central Punjab, Lahore, Pakistan.
- Member of Organizing Committee at "One day technical workshop on ENDNOTE" organized by Department of Basic and Applied Chemistry, Faculty of Science and Technology, University of Central Punjab, Lahore on 28th September, 2022.
- "Entrepreneurship in Biochemistry & Molecular Biology" on 3rd August 2022 organized by Department of Basic & Applied Chemistry at University of Central Punjab, Lahore.
- Effectiveness of Virtual Learning organized by Department of Biochemistry at University of Central Punjab, Lahore.
- Lab Management Training of faculty of Life Sciences during March 21st – 22nd 2022 at University of Central Punjab, Lahore.
- "One Day Training Session for Diabetes Advanced Diagnosis Techniques, Management, and Treatment" conducted by Department of Biochemistry in collaboration with Society of Life Sciences and Dilawar Hussain Foundation on November 18th 2021 at University of Central Punjab.
- Lab Orientation Workshop at Faculty of Life Sciences during August 25th – 26th 2021 at University of Central Punjab, Lahore.
- 6th International Conference on Drug Development – Natural & Synthetic "Current Approaches and Emerging Trends for the Development and Discovery of Drugs" (29-30 November, 2019) organized by Centre for Advanced Drug Research, COMSATS University Islamabad, Abbottabad Campus.
- 1st International Conference on "Advancements in Biotechnology & Biocomputing" organized by Department of Biological Sciences, International Islamic University, Islamabad during 7-9 February, 2019.
- 5th International Conference on Drug Development – Natural & Synthetic "Current Approaches and Emerging Trends for the Development and Discovery of Drugs" (28-29 June, 2018) organized by Centre for Advanced Drug Research, COMSATS University Islamabad, Abbottabad Campus.

- 13th Biennial Conference on "Recent Advances & Challenges in Molecular Biology, Biochemistry and Biotechnology" (25-27 August, 2016) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- 2nd International Symposium on "Drug Development- Natural & Synthetic" (23-25 August, 2015) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- DAAD-HEC International Summer School "Challenges in Molecular Medicine and Drug Research" (1-3 September, 2014) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- Three days Workshop on "DNA Sequencing" (10-12 February, 2014) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.
- 1st International Symposium on "Drug Development- Natural & Synthetic" (25-27 August, 2013) organized by Centre for Advanced Drug Research, COMSATS, Abbottabad.

(j) Workshops as Resource Person

1. "7th One-Day Lab Introductory Hands-on-Training/workshop of Department of Basic and Applied Chemistry on 23rd April, 2025.
2. "6th One-Day Lab Introductory Hands-on-Training/workshop of Department of Basic and Applied Chemistry on 3rd October, 2024.
3. One day hands on training on "Computational Drug Designing" at University of Veterinary and Animal Sciences held on 30th October, 2023.
4. "5th 2 days lab orientation and hands on training/workshop" for the research students of the department of Basic and Applied Chemistry on 1st August 2023 to 2nd August 2023.
5. "4th 1-Day Lab Orientation & Hands-on-Training/workshop for Biochemistry Research Students" conducted by Department of Basic & Applied Chemistry on 22nd March, 2023.
6. The 3rd two-days Lab Orientation and hands on training/ Workshop for Biochemistry Research Students organized by Department of Basic & Applied Chemistry held in October, 2022.
7. The one-day virtual webinar on "Targeting Serine Protease Enzymes for the Discovery of Novel Inhibitors to Combat COVID-19" organized by BioSolveIT in 2022.
8. The one-day Training on "Immunoinformatics" organized by Institute of Pharmaceutical Sciences, University of Veterinary and Animal Sciences held on November 01, 2022.
9. The one-day Hands on workshop on "Bioinformatics: Converting knowledge to data" organized by The Centre for Advanced Drug Research (CADR) COMSATS University, Abbottabad Campus on 7th October, 2019.
10. The one-day Hands on workshop on "Pharmacophore Modelling and Virtual Screening" organized by The Centre for Advanced Drug Research (CADR) COMSATS University, Abbottabad Campus on 14th January, 2019.
11. The one-day Hands on workshop on "Computational Methods for Drug Design and Discovery" was organized by the Centre for Advanced Drug Research (CADR) COMSATS University, Abbottabad Campus on 20th November, 2018.

(k) University Service

- Started MPhil in Chemistry and Ph.D. in Chemistry at University of Central Punjab in 2024
- Board of Studies, Advisory board member, University of Central Punjab, Pakistan, (2022-present)

- Board of Faculty, Advisory board member, University of Central Punjab, Pakistan, (2022-present)
- Ethical review board, Committee member, University of Central Punjab, Pakistan, (2022-present)
- Board of Advanced Studies and Research (BASR), Committee member, University of Central Punjab, Pakistan, (2022-present)
- Purchase committee member, University of Central Punjab, Pakistan, (2022-present)
- Member of Board of Studies, International Islamic University, Islamabad, Pakistan
- Member of Lab Management Committee, University of Central Punjab, Pakistan, (2021-present)

(l) Service to Profession/Industry

- Esteem Pharmaceuticals, Pakistan, Consultancy, (2022-present)
- Department of Clinical Neuroscience, University of Calgary, Canada, Consultant Research Fellow.

(m) Memorandum of Understanding (MoU)

- Department of Medicinal Chemistry at the College of Pharmacy, University of Sharjah, UAE, **2023**.
- NovaMed Pharmaceuticals, Lahore, Pakistan, **2022**.

(n) Public Service

N/A

7. List of Publications *(in chronological order, starting with most recent)*

(a) International Refereed Journals *(Published)*

1. Taqueer Salman, Mohsin Javed, **Sumera Zaib** et al. Effect of different concentrations of Bismuth Molybdate as an electrocatalyst for water splitting and antibacterial activity. Microscopy Research and Technique, **IF=2.5**
2. Anil Ravi, **Sumera Zaib***, Shabab Zahra, Imtiaz Khan, Hafiz Saqib Ali, Mohammed I El-Gamal, Hanan S Anbar, 2025. Synthesis, in vitro and in vivo evaluation, and computational modeling analysis of thioxothiazolidine derivatives as highly potent and selective α -amylase inhibitors. European Journal of Medicinal Chemistry, 291, p.117584. **IF=6.7**
3. **Sumera Zaib***, Nehal Rana, Hafiz Saqib Ali, Mujeeb ur Rehman, Nasser S Awwad, Hala A Ibrahim, Imtiaz Khan, 2025. Identification of potential inhibitors targeting yellow fever virus helicase through ligand and structure-based computational studies. Journal of Biomolecular Structure and Dynamics, 43(6), pp.3031-3048. **IF = 5.235**
4. Nafeesa Naeem, **Sumera Zaib***, Ehsan Ullah Mughal, Gehan Ahmed Othman, Amina Sadiq, Nehal Rana, 2025. Discovery of bis-chalcones and bis-pyrimidines as potential

- urease inhibitors: from synthesis to computational insights. *Future Medicinal Chemistry*, 17(8), pp.929-941. **IF= 3.7**
5. **Sumera Zaib***, Hira Javed, Nehal Rana, Zainab Zaib, Shahid Iqbal, Imtiaz Khan. 2025. Therapeutic chemoresistance in ovarian cancer: emerging hallmarks, signaling mechanisms and alternative pathways. *Current Medicinal Chemistry*, 32(5), pp.923-938. **IF=4.1**
 6. **Sumera Zaib***, Imtiaz Khan, Laiba Babar, Nawal Naseer, Danial Nadeem, Ravish Fatima, Ayed A Dera, Fadi Jaber, KK Mujeeb Rahman, 2025. Isolation and Characterization of an Insulin-Like Protein From *Moringa Oleifera* and Estimation of Its Antidiabetic Potential. *ChemistrySelect*, 10(6), p.e202401991. **IF= 2.307**
 7. **Sumera Zaib***, Imtiaz Khan, Aliya Ibrar, Hafiz Saqib Ali, Nehal Rana, Rubina Munir, Shabab Zahra, Abdel-Basit Al-Odayni, Christopher John McAdam, Tuncer Hökelek, Antonio Frontera. 2025. Synergistic effect of hydrogen bonding and C-H... n interactions to modulate the supramolecular assemblies of isobenzofuranones: X-ray crystallography, DFT analysis and antihyperglycemic potential. *Journal of molecular structure*, 1321, p.140263. **IF= 4.0**
 8. **Sumera Zaib***, Hira Javed, Nehal Rana, Zainab Zaib, Shahid Iqbal, Imtiaz Khan, 2025. Therapeutic chemoresistance in ovarian cancer: emerging hallmarks, signaling mechanisms and alternative pathways. *Current Medicinal Chemistry*, 32(5), pp.923-938. **IF = 4.1**
 9. Arif Malik, Mehreen Hassan, Sulayman Waquar, Muhammad Wasim, Anam Naz, Faryal M Awan, Muhammad T Khan, Ali I Khawaja, **Sumera Zaib**, Jamshed Iqbal, Ayesha Zahid, Marvi Marvi, Javeid Iqbal, Heng Wang, Dong-Qing Wei, 2025. Neuroprotective role of epigallocatechin-3-gallate, albeginin and melanoxetin in alzheimer's disease. *Phytomedicine Plus*, 5(1), p.100740. **IF= 3.7**
 10. Asma Arshad, **Sumera Zaib**, 2024. Evaluation haematological parameters with liver enzymes and renal dysfunction markers in Beta-thalassemia major patients, *Journal of Population Therapeutics and Clinical Pharmacology*, 1175-1181. **IF= 0.3**
 11. Muhammad Sarfraz, Khurram Waqas, Hamid Saeed Shah, Faisal Usman, Tariq Ismael, **Sumera Zaib***, Riffat Khan, Zobia Jawad, Yasser Shahzad, 2024. Hyaluronic acid functionalized chitosan nanoparticles for the delivery of ellagic acid to breast cancer cells: Fabrication, characterization and pharmacological assessment. *Journal of Drug Delivery Science and Technology*, 102, p.106418. **IF= 4.5**
 12. Muhammad Akash, Nehal Rana, Sana Aslam, Matloob Ahmad, Muhammad Jawwad Saif, Aneeza Asghar, Sadia Sultan, Sami A Al-Hussain, Afifa Liaqat, **Sumera Zaib***, Magdi EA Zaki. 2024. Pyridylpiperazine-based carbodithioates as urease inhibitors: synthesis and biological evaluation. *Frontiers in Chemistry*, 12, p.1423385. **IF= 3.8**

13. **Sumera Zaib***, Imtiaz Khan, Aliya Ibrar, Christopher John McAdam, Safaa N Abdou, Mohamed M Ibrahim, Salah M El-Bahy, Antonio Frontera, 2024. Energetic features of H-bonded and antiparallel n-stacked supramolecular assemblies in pyrazolones: Experimental, computational and biological analyses. *Journal of molecular structure*, 1318, p.139232. **IF**= 4.0
14. **Sumera Zaib***, Shabbir Ahmad, Imtiaz Khan, Yousef A Bin Jordan, Gezahign Fentahun Wondmie, 2024. An evaluation of inflammatory and endothelial dysfunction markers as determinants of peripheral arterial disease in those with diabetes mellitus. *Scientific Reports*, 14(1), p.15348. **IF**= 3.8
15. **Sumera Zaib***, Imtiaz Khan, Aliya Ibrar, Nehal Rana, Hafiz Saqib Ali, Christopher John McAdam, Rosa M Gomila, Islam H El Azab, MHH Mahmoud, Zeinhom M El-Bahy, Antonio Frontera, 2024. Hydrogen bonding, halogen bonding and C-H... n interactions governing the supramolecular architecture of 1-(4-(4-bromophenyl) piperazin-1-yl)-2-chloroethan-1-one: Insights from X-ray crystallography, DFT calculations and urease inhibitory assessment. *Journal of molecular structure*, 1317, p.139065. **IF** = 4.0
16. Ahmad Hassan, **Sumera Zaib***, Tehmina Anjum, 2024. Evaluation of antifungal potentials of Albizia kalkora extract as a natural fungicide: In vitro and computational studies. *Bioorganic Chemistry*, 150, p.107561. **IF** = 5.1
17. Omar Hashem, **Sumera Zaib***, Seyed-Omar Zariaei, Hira Javed, Reena A Kedia, Hanan S Anbar, Imtiaz Khan, Anil Ravi, Mohammed I El-Gamal, Ghalia Khoder, 2024. Design and discovery of urease and Helicobacter pylori inhibitors based on benzofuran/benzothiophene-sulfonate and sulfamate scaffolds for the treatment of ureolytic bacterial infections. *International Journal of Biological Macromolecules*, 271, p.132502. **IF** = 8.2
18. **Sumera Zaib***, Imtiaz Khan, Hafiz Saqib Ali, Muhammad Tayyab Younas, Aliya Ibrar, Abdel-Basit Al-Odayni, Abdullah A Al-Kahtani, 2024. Design and discovery of anthranilamide derivatives as a potential treatment for neurodegenerative disorders via targeting cholinesterases and monoamine oxidases. *International Journal of Biological Macromolecules*, 272, p.132748. **IF** = 8.2
19. Rubina Munir, **Sumera Zaib***, Muhammad Zia-ur-Rehman, Hira Javed, Ayesha Roohi, Muhammad Zaheer, Nabiha Fatima, Mashooq Ahmad Bhat, Imtiaz Khan, 2024. Exploration of morpholine-thiophene hybrid thiosemicarbazones for the treatment of ureolytic bacterial infections via targeting urease enzyme: Synthesis, biochemical screening and computational analysis. *Frontiers in Chemistry*, 12, p.1403127. **IF** = 3.8
20. Ali Imran Khawaja, Sampath Chinnam, Zaheer Ahmad, Humayun Riaz, Basappa C

- Yallur, Arif Malik, Khawaja Danial Hassan, Bushra Khalid, Abdul Qaddoos, Waqas Ahmad, **Sumera Zaib**, 2024. Remyelinating potential of *Olea Europaea* and *Arachis Hypogaea* on Experimental autoimmune Encephalomyelitic model of Multiple Sclerosis by downregulating the pro-inflammatory cytokines, Preprint.
21. Atteeque Ahmed, **Sumera Zaib**, Mashooq Ahmad Bhat, Aamer Saeed, Muhammad Zain Altaf, Fatima Tuz Zahra, Ghulam Shabir, Nehal Rana, Imtiaz Khan, 2024. Acyl pyrazole sulfonamides as new antidiabetic agents: synthesis, glucosidase inhibition studies, and molecular docking analysis. *Frontiers in Chemistry*, 12, p.1380523. **IF= 3.8**
 22. Lutf Ullah Zahid, **Sumera Zaib**, Aamer Saeed, Hussam Alharbi, Majed S. Aljohani, Osama Alharbi, Nehal Rana, Imtiaz Khan, Ghulam Shabir, Atteeque Ahmed, Arslan Saleem, Nasser S Awwad, Hala Ibrahim, 2024. Synthesis, glucosidase inhibition, and in silico modeling analysis of highly fluorinated 2-imino-1, 3-thiazolines in search of potent antidiabetic agents. *ACS omega*, 9(13), pp.15603-15614. **IF = 4.1**
 23. Muhammad Akash, **Sumera Zaib**, Dr. Matloob Ahmad, Sadia Sultan, Sami A. Al-Hussain, 2024. Synthesis and biological evaluation of pyridylpiperazine hybrid derivatives as urease inhibitors. *Frontiers in Chemistry*, 12, p.1371377. **IF = 3.8**
 24. Atteeque Ahmed, **Sumera Zaib***, Aamer Saeed, Muhammad Zain Altaf, Fatima Tuz Zahra, Ghulam Shabir, Nehal Rana, Imtiaz Khan, Hanan A. Ogaly, Fatimah AM Al-Zahrani. 2024. Acyl pyrazole sulfonamides as new antidiabetic agents: synthesis, glucosidase inhibition studies, and molecular docking analysis. *Frontiers in Chemistry*, 12, p.1380523. **IF= 4.1**
 25. **Sumera Zaib**, Rubina Munir, Imtiaz Khan, Noman Javid, Rahila Huma, Uzma Mustafa, Nehal Rana, Christopher John McAdam, Colleen Hui Shiuan Yeow, Jonathan M White, Tuncer Hökelek, Khalid M Alotaibi, Matar Alshalwi, Antonio Frontera, 2024. Supramolecular networks featuring diverse array of noncovalent interactions in crystals of hydrazinylidene-benzothiazinediones: X-ray crystallographic, DFT and biochemical analysis. *Journal of molecular structure*, 1306, p.137840. **IF = 4.0**
 26. **Sumera Zaib***, Aqsa Hayyat, Imtiaz Khan, 2024. Nutritional and health benefits of cereals and grains. *Current Nutrition & Food Science*, 20(10), pp.1205-1221. **IF = 0.9**
 27. Hamid Saeed Shah, **Sumera Zaib**, Faisal Usman, Muhammad Sarfraz, Rabia Faiz, Saira Abdul Rehman, Azmat Ali Khan, Amer M Alanazi, Riffat Khan, Usman Narullah, Imran Nazir, 2024. Synthesis, characterization, pharmacological and computational evaluation of hyaluronic acid modified chebulinic acid encapsulated chitosan nanocomposite for cancer therapy. *International Journal of Biological Macromolecules*, 263, p.130160. **IF = 8.2**

28. Feroz Khan, Sarmir Khan, Nehal Rana, Tariq Rahim, Abida Arshad, Imtiaz Khan, Hanan A Ogaly, Dalia Abd El Moneim Ahmed, Ayed A Dera, **Sumera Zaib***, 2024. Mutational analysis of consanguineous families and their targeted therapy against dwarfism. *Journal of Biomolecular Structure and Dynamics*, pp.1-18. **IF = 5.235**
29. Shabab Zahra, **Sumera Zaib***, Imtiaz Khan, 2024. Identification of isobenzofuranone derivatives as promising antidiabetic agents: Synthesis, in vitro and in vivo inhibition of α -glucosidase and α -amylase, computational docking analysis and molecular dynamics simulations. *International Journal of Biological Macromolecules*, 259, p.129241. **IF = 8.2**
30. **Sumera Zaib**, Aqsa Hayat, Imtiaz Khan, 2024. Probiotics and their beneficial health effects. *Mini reviews in medicinal chemistry*, 24(1), pp.110-125. **IF= 3.8**
31. Rubina Munir, **Sumera Zaib**, Imtiaz Khan, Amna Yousaf, Christopher John McAdam, Colleen Hui Shiuan Yeow, Jonathan M White, Tuncer Hökelek, Nasser S Awwad, Hala A Ibrahim, Antonio Frontera, 2024. Cooperative assemblies featuring hydrogen bonding and CH... π interactions in 2-(methanesulfonamido) benzohydrazide derivatives: Experimental, computational and biochemical assessment. *Journal of Molecular Structure*, 1295, p.136752. **IF = 3.8**
32. **Sumera Zaib**, Areeba, Imtiaz Khan, 2024. Purinergic signaling and its role in the stem cell differentiation. *Mini Reviews in Medicinal Chemistry*, 24(8), pp.863-883. **IF= 3.8**
33. Fiby N Takla, **Sumera Zaib**, Waleed A Bayoumi, Kiran Shehzadi, Shahenda M El-Messery, Sharjeel Anjum, Amir Faisal, Magda NA Nasr, 2024. Targeting carbonic anhydrases II/IX/XII with novel series of coumarin-based compounds: Synthesis, biological activity and molecular dynamics analysis. *Journal of Molecular Structure*, 1300, p.137277. **IF = 3.8**
34. Lutf ullah Zahid, **Sumera Zaib,*** Aamer Saeed,* Nehal Rana, Ghulam Shabir, Atteeque Ahmad, Arslan Saleem, Imtiaz Khan, Hanan A. Ogaly and Fatimah AM Al-Zahrani. 2024. Synthesis, glucosidase inhibition, and in silico modeling analysis of highly fluorinated 2-imino-1, 3-thiazolines in search of potent antidiabetic agents. *ACS omega*, 9(13), pp.15603-15614. **IF=4.1**
35. **Sumera Zaib**, Hamid Saeed Shah, Imtiaz Khan, Huma Riaz, Zobia Jawad, Hafiz Muhammad Mazhar Asjad, Memoona Ishtiaq, Hanan A. Ogaly, Gehan Othman, Dalia Abd El Moneim Ahmed. 2024. Fabrication and evaluation of anticancer potential of diosgenin incorporated chitosan-silver nanoparticles; in vitro, in silico and in vivo studies. *International Journal of Biological Macromolecules*, 254, p.127975. **IF = 8.2**
36. Rubina Munir, Imtiaz Khan, Leena Siddiqui, Noman Javid, Muhammad Zia-ur-Rehman, Hafiz Saqib Ali, Memoona Saeed, **Sumera Zaib**, Nasser S. Awwad, Hala A.

- Ibrahium , Colleen Hui Shiuan Yeow, Jonathan M. White, Ayed A. Dera. 2024. Regioselective metal-free synthesis of sulfostyryl-quinoline hybrid framework: Experimental and computational mechanistic insights. *Journal of Molecular Structure*, 1315, p.138894. **IF= 3.8**
37. Rubina Munir, **Sumera Zaib**, Imtiaz Khan, Amna Yousaf, Christopher John McAdam, Colleen Hui Shiuan Yeow, Jonathan M. White, Tuncer Hökelek, Nasser S. Awwad, Hala A. Ibrahium, Antonio Frontera. 2024. Cooperative assemblies featuring hydrogen bonding and CH... π interactions in 2-(methanesulfonamido) benzohydrazide derivatives: Experimental, computational and biochemical assessment. *Journal of Molecular Structure*, 1295, p.136752. **IF= 3.8**
 38. Gabriel O Anyanwu, Uju D Ejike, Gideon A Gyebi, Khalid Rauf, Jamshed Iqbal, **Sumera Zaib**, Usunomena Usunobun, Eusebius C Onyeneke, Badriyah S Alotaibi, Gaber El-Saber Batiha. 2023. Phytochemical analysis, in vitro and in silico effects from *Alstonia boonei* De Wild stem bark on selected digestive enzymes and adipogenesis in 3T3-L1 preadipocytes. *BMC complementary medicine and therapies*, 23(1), p.370. **IF = 2.838**
 39. F Ullah, I Ahmad, S Zaib, M Abrar, M Khalil, MAMA Ebdah, SM Ramay, M Saleem. 2023. A comprehensive study on Ni-Doped cobalt ferrites for optical response and anti-bacterial activity. *Digest Journal of Nanomaterials & Biostructures (DJNB)*, 18(3). **IF = 0.963**
 40. Hamid Saeed Shah, **Sumera Zaib***, Imtiaz Khan, Kiran Shahzadi, Sajjad Awan, Zobia Jawad, Nasser S. Awwad, Hala A. Ibrahium. 2023. Preparation and investigation of a novel combination of *Solanum nigrum*-loaded, arabinoxylan-cross-linked β -cyclodextrin nanosponges for the treatment of cancer: in vitro, in vivo, and in silico evaluation. *Frontiers in Pharmacology*, 14, p.1325498. **IF = 8.2**
 41. Muhammad Tayyab Younas, **Sumera Zaib,*** Imtiaz Khan. 2023. Discovery of Hydrazone Scaffolds as Potent and Selective Multitarget-Directed Ligands for the Treatment of Neurodegenerative Disorders. *ChemistrySelect*, 8(47), p.e202303089. **IF=2.307**
 42. **Sumera Zaib**, Nehal Rana, Nadia Hussain, Areeba Areeba, Hanan A. Ogaly, Fatimah AM Al-Zahrani, Imtiaz Khan, 2023. Discovery of druggable potent inhibitors of serine proteases and farnesoid X receptor by ligand-based virtual screening to obstruct SARS-CoV-2. *International Journal of Biological Macromolecules*, 253, p.127379. **IF= 8.2**
 43. Hamid Saeed Shah, **Sumera Zaib**, Muhammad Sarfraz, A Alhadhrami, Mohamed M Ibrahim, Aamir Mushtaq, Faisal Usman, Memoona Ishtiaq, Muhammad Sajjad, Hafiz Muhammad Mazhar Asjad, Umar Farooq Gohar, 2023. Fabrication and evaluation of

- anticancer potential of eugenol incorporated chitosan-silver nanocomposites: in vitro, in vivo, and in silico studies. *AAPS PharmSciTech*, 24(6), p.168. **IF= 3.3**
44. **Sumera Zaib**, Muhammad Tayyab Younas, Imtiaz Khan, Hafiz Saqib Ali, John McAdam, Jonathan M. White, Fadi Jaber, Nasser S. Awwad, Hala A. Ibrahim, 2023. Pyrimidine-morpholine hybrids as potent druggable therapeutics for Alzheimer's disease: Synthesis, biochemical and in silico analyses. *Bioorganic chemistry*, 141, p.106868. **IF= 5.1**
45. Ayed A. Dera, **Sumera Zaib**, Areeba Areeba, Nadia Hussain, Nehal Rana, Hira Javed, Imtiaz Khan, 2023. Identification of potent inhibitors targeting EGFR and HER3 for effective treatment of chemoresistance in non-small cell lung cancer. *Molecules*, 28(12), p.4850. **IF= 4.6**
46. **Sumera Zaib**, Hira Javed, Imtiaz Khan, Fadi Jaber, Ali Sohail, Zainab Zaib, Tooba Mehboob, Naila Tabassam, Hanan A Ogaly, 2023. Neurodegenerative diseases: their onset, epidemiology, causes and treatment. *ChemistrySelect*, 8(20), p.e202300225. **IF= 2.307**
47. Afnan I. Shahin, **Sumera Zaib**, Seyed-Omar Zaraei, Reena A. Kedia, Hanan S. Anbar, Muhammad Tayyab Younas, Taleb H. Al-Tel, Ghalia Khoder, and Mohammed I. El-Gamal, 2023. Design and synthesis of novel anti-urease imidazothiazole derivatives with promising antibacterial activity against *Helicobacter pylori*. *PLoS One*, 18(6), p.e0286684. **IF= 3.752**
48. Rubina Munir, **Sumera Zaib**, Imtiaz Khan, Zirwa tul Islam, Rosa M Gomila, Christopher John McAdam, Colleen Hui Shiuan Yeow, Jonathan M White, Tuncer Hökelek, Abdulaziz A Al-Askar, Eslam B Elkaeed, Antonio Frontera, 2023. Complex interplay of hydrogen bonding, halogen bonding and n-interactions in methyl 2-(7-chloro-1H-pyrazolo [3, 4-b] quinolin-1-yl) acetate: Synthesis, X-ray crystallography, energetic features and anti-urease efficacy. *Journal of Molecular Structure*, 1287, p.135625. **IF= 3.8**
49. **Sumera Zaib**, Aliya Ibrar, Imtiaz Khan, Nehal Rana, Rosa M. Gomila, Christopher John McAdam, Abdulaziz A. Al-Askar, Eslam B. Elkaeed, Antonio Frontera, 2023. Insight into structural topology and supramolecular assembly of tetrahydrocarbazole-carbonitrile: On the importance of noncovalent interactions and urease inhibitory profile. *Journal of molecular structure*, 1285, p.135522. **IF= 3.8**
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