



# **Online Meeting on Recent Developments in Drug Discovery and Medicinal Chemistry**

**Organized by COMSTECH**

**in collaboration with**

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

**Mode of the Workshop (ON-LINE)**

**26-27 July, 2021**

# Program

**Day-1 (26<sup>th</sup> July 2021) – Monday**  
(Timing according to Pakistan Standard Time)

## Inaugural Session

09:00 - 09:30	<b>Registration</b>
09:30-09:35	<b>Recitation of the Holy Quran</b>
09:35-09:40	<b>Welcome Remarks</b> <b>Ms. Khazima Muazim</b> <b>Program Manager, COMSTECH</b>
09:40-10:00	<b>Welcome and Keynote Address</b> <b>H.E. Prof. Dr. M. Iqbal Choudhary</b> <i>H. I., S. I., T. I.</i> <b>Coordinator General, COMSTECH</b>
10:00-10:05	<b>Vote of Thanks</b> <b>Dr. Hina Siddiqui</b> <b>Associate Professor ICCBS</b>
10:10-11:30	<b><i>An Overview of Prodrugs</i></b> <b>Prof. Dr. Keykavous Parang,</b> <b>University of Chapman, USA</b>
11:30-12:30	<b><i>Medicinal Chemistry of New <math>\alpha</math>-Glucosidase and <math>\alpha</math>-Amylase Inhibitors</i></b> <b>Prof. Dr. Khalid M. Khan</b> <i>S. I., T. I.</i> <b>ICCBS, University of Karachi, Pakistan</b>
12:30-13:30	<b><i>Metal-based Antitumor Agents of Traditional Chinese Medicines Active Ingredients and Their Derivatives</i></b> <b>Prof. Dr. Zhen-Feng Chen</b> <b>Guangxi Normal University, P. R. China</b>
<b>13:30 – 1400</b>	<b>Lunch and Prayer Break</b>
14:00-15:00	<b><i>Modern Drug Discovery and Medicinal Chemistry</i></b> <b>Dr. Muhammad Saeed</b> <b>Lahore University of Management Sciences, Pakistan</b>
15:00-16:00	<b><i>Investigation of Natural Medicines for Covid-19</i></b> <b>Assoc. Prof. Dr. Mustafa Güzel</b> <b>Istanbul Medipol University, Turkey</b>

<b>Day-2 (27<sup>th</sup> July 2021) -Tuesday</b>	
09:30-10:30	<i>Discovery and Pharmacological Evaluation of a Novel Series of Adamantyl Thiourea as G-protein Coupled Receptor Antagonists</i> <b>Prof. Dr. Jamshed Iqbal, T.I., FRSC</b> COMSATS University Islamabad, Pakistan
10:30-11:30	<i>Examples of Medicinal Chemistry Research: Small Molecule from Chinese Herbal Medicine</i> <b>Prof. Dr. Hengshan Wang</b> Guangxi Normal University, P. R. China
11:30-12:30	<i>The Development on Potential Metal-Based Veterinary Drugs with Improved Efficacies than Fluoroquinolones</i> <b>Prof. Dr. Yancheng Liu</b> Guangxi Normal University, P. R. China
<b>12:30-13:00</b>	<i>Lunch and Prayer Break</i>
13:00-14:00	<i>Targeting Viral Proteases for Designing and Discovering Direct-Acting Antivirals (DAAs)</i> <b>Dr. Muhammad Saeed</b> Lahore University of Management Sciences, Pakistan
14:00-15:00	<i>Computational Tools and Techniques for Early Phase of Drug Discovery Research</i> <b>Dr. Reaz Uddin</b> ICCBS, University of Karachi, Pakistan
15:00-16:00	<i>Case Studies: Successful Drug Discovery Made through the Medicinal Chemistry Approach</i> <b>Dr. Hina Siddiqui</b> ICCBS, University of Karachi, Pakistan
16:00-16:30	<b>Closing Session</b>

# Profiles of the Speakers

(Note: Profiles are arranged according to the order of their lectures)

## Prof. Dr. Keykavous Parang,

**Affiliation:** Associate Dean of Research, Innovation, and Global Affairs,  
Professor of Medicinal Chemistry and Pharmacology  
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Prof. Dr. Parang is Associate Dean of Research, Innovation, and Global Affairs and a Full Professor of Medicinal Chemistry and Pharmacology at Chapman University School of Pharmacy in Irvine, California. He earned a Pharm. D. degree from Tehran University of Medical Sciences in 1989. He received his Ph.D. in medicinal chemistry from the Faculty of Pharmacy at the University of Alberta in 1997, followed by a postdoctoral study in the field of solid-phase organic synthesis in the Department of Chemistry, University of Alberta. He pursued additional postdoctoral studies at Rockefeller University in New York and Johns Hopkins University in Baltimore in bioorganic chemistry. He joined the University of Rhode Island in October 2000 and became a full professor in July 2008. He served as the Program Coordinator of Rhode Island IDeA Network of Biomedical Research Excellence (RI-INBRE) NIH program (2012-2013). He joined Chapman University to assist in establishing the School of Pharmacy. He is an author of 189 peer-reviewed publications, 10 patents, and 171 meeting abstracts. His specific research areas currently under investigation include (1) using peptides as cell-penetrating molecular transporters in drug delivery; (2) designing protein kinase inhibitors; (3) developing multifunctional antiviral, anticancer, and antibacterial agents; and (4) designing peptide nanomaterials for nanomedicine. One major area currently under investigation is to design peptide nanomaterials for applications in drug delivery. The objective of this project is to design and evaluate

peptide nanomaterials as cell-penetrating nuclear targeting agents or molecular transporters of bioactive cell-impermeable compounds. This study will document the potential for new hybrid peptide-drug assemblies that may be used for the non-covalent or covalent targeted delivery of bioactive molecules, including cell-impermeable compounds with biological significance. He is an author of 205 peer-reviewed publications, 13 issued or pending patents, and more than 180 meeting abstracts.

## **Prof. Dr. Zhenfeng Chen**

**Affiliation:** Director, State Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources, School of Chemistry and Pharmacy, Guangxi Normal University, Guilin 541004, P. R. China

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Prof. Chen received his Ph.D. in Inorganic Chemistry from Nanjing University of China in 2001. Then he worked in Guangxi Normal University of China as an associate professor. In 2003, he became a professor with a research focus on medicinal chemistry. In 2004, he was the owner of Program for New Century Excellent Talents in University of Chinese Ministry of Education; the Second Level Owner of Program for New Century Ten, Hundred, Thousand Distinguished Talent of Guangxi of P. R. China. In 2011, he became the Bagui Scholar of Guangxi Zhuang Autonomous Region in China. In 2012, he was approved as the Leader of Innovation Team of Ministry of Education of China. In 2015, he was the Owner of Program for National Hundred, Thousand and Ten Thousand Talent and National outstanding contribution and experts of China. In 2016, he was approved to receive the State Council special allowance. Currently, he is Executive Vice Dean of State Key Laboratory of State Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources at Guangxi Normal University of China. He has completed five NNSF of China, one 973 Project and two Innovation Team Project of the Ministry of Education of China and published more about 230 SCI papers in peer-reviewed journals, one book chapter, and is the inventor of 53 authorized patents. Dr. Chen's major research interest is drug discovery in the fields of traditional Chinese medicine active ingredients metal-based anticancer agents.

**Prof. Dr. Khalid Mohammed Khan** *T. I., S. I.*

Ph. D. (Kar.), Postdoc. (Germany)

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

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Prof. Dr. Khan is among the most prominent scientists of Pakistan recognized for his original contributions in the field of medicinal chemistry and drug discovery. He has received many prestigious awards and honours, including Pakistan Academy of Sciences Gold Medals 2004, and 2010. Most Cited Paper 2005-2008 Award from Elsevier Publishers, Amsterdam, Netherlands. The President of Pakistan has awarded civil awards Tamgha-i-Imtiaz and Sitara-i-Imtiaz in recognition of his contributions in medicinal chemistry in 2005 and 2012, respectively. He is also Recipient of Research Productivity Awards (RPA) 2001-2017 from the Pakistan Council for Science & Technology (PCST) in recognition of his high-quality research. He established a world class medicinal and synthetic laboratory at the HEJ Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, focusing on discovery of new enzyme inhibitors and other bioactive compounds. He is mentoring a large number of young researchers in the field of drug designing and drug and designing. He supervised and co-supervised 90 Ph. D./MS/M. Phil. scholars. In last two decades, he enriched world literature with several novel classes of bioactive substances, and helped in the development of new pharmacophores. The major emphasis of his work is on the synthesis of inhibitors of clinically important enzymes. In this work, he uses a minimum pharmacophore approach and concentrates on the understanding of the functional profile of the active parts of potential drug candidates. He has rationally designed a number of new lead compounds which are active against diabetes, and peptic ulcer. Detailed experimental studies on these compounds are in progress. He is also pioneer of microwave-assisted synthetic chemistry in Pakistan. An important facet of Dr. Khan's scientific work is the development of new synthetic methodologies, and facile organic transformations. His current research interests also include bioassay-directed isolation of natural products and development of nano-medicines. He is co-editor of two books several chapters in books. He has authored or co-authored over 800 research papers published in the journals of international repute. He has cumulative impact factor over 1545, and citation index exceeding 17,000 and seventeen (18) international and national patents representing top quality research productivity.

## **Assoc. Prof. Dr. Mustafa Güzel**

**Affiliation:** Director of Drug Discovery and Development Research Center, Istanbul Medipol University, Turkey

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Assoc. Prof. Dr. Guzel graduated from Hacettepe University School of Engineering, Ankara, Turkey with a B. Sc. degree in Chemistry in 1987 and completed his M. Sc. and Ph. D. Degrees on Organic/Medicinal Chemistry at Clemson University, Clemson (USA), in 1996 and 2001, respectively. He worked as organic lab coordinator at Northeastern University and later joined to ArQule Inc. as Sr. Synthetic Organic Chemist upon his graduation. He then joined TransTech Pharma Inc. in High Point, NC (USA) and assumed various positions in Medicinal Chemistry Department between 2001 and 2014. In 2014 he started working as an Assistant Professor at International School of Medicine in Department of Medical Pharmacology at Istanbul Medipol University. In 2017 he was promoted to an Associate Professor in medical pharmacology acting as a chair. In 2019 he was appointed as the department chair of Molecular Medicine and Biotechnology. In January 2020, he then became the Director of Drug Discovery and Development Research Center in newly established Health Sciences and Technologies Research Institute, currently leading two critical drug development projects for Covid-19 with a local pharma company as well as several domestic and European granted drug discovery projects in Molecular Discovery and Development laboratories of the university.

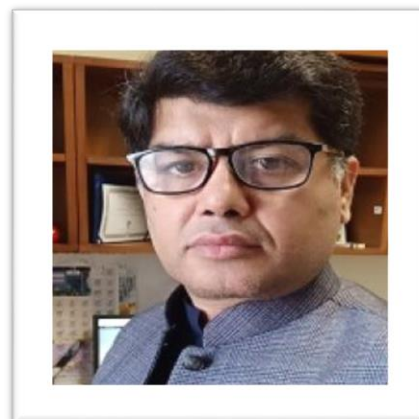
## Dr. Muhammad Saeed

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Dr. Muhammad Saeed Joined LUMS in 2014 as an Associate Professor. He established the Bioorganic and Medicinal Chemistry (BMC) group in the Department of Chemistry and Chemical Engineering. Originally trained as synthetic organic chemist, he has extensive postdoctoral research experience at the interface of chemistry and biology. He is interested to address the modern challenges in biological sciences and medicinal chemistry by using the tools of organic chemistry. More specifically, he pursues rational antiviral and anticancer drug designing and discovery by using modern day techniques of computational modeling, protein dynamics and simulations, supported by the conventional wet-chemistry of organic synthesis and high-throughput screening of synthetic compounds and natural products.

Dr. Saeed received his Ph. D. degree in organic chemistry from Eberhard-Karls University of Tuebingen, Germany under the supervision of Prof. Dr. Dr (hc mult) Wolfgang Voelter, after accomplishing total syntheses of several natural products and medicinal analogs using the chirality and topology of abundant carbohydrates. After Ph. D., he joined the research group of Prof. Ercole Cavalieri, DSc at the Eppley Cancer Institute, University of Nebraska Medical Center, Omaha, USA, where he participated as chemical biologist in mechanistic investigation of cancer initiation by estrogens and related carcinogenic compounds. Before joining LUMS, he has also spent some time in the Department of Chemistry, University of Iowa, where he worked as a visiting assistant professor as well as conducted research as postdoctoral scholar with Prof. Amnon Kohen, D. Sc. in the area of development of radiopharmaceuticals as positron emission tomography (PET) tracers. He has published around 50 research articles in reputed international journals. His is currently investigating proteases of different viruses (COVID-19, dengue, HCV) as drug targets for designing efficient direct-acting antivirals (DAAs).

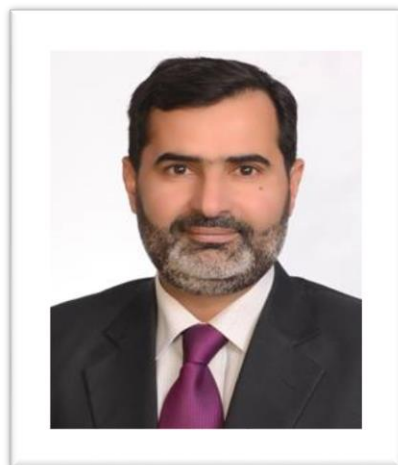


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Prof. Dr. Jamshed Iqbal is Chairman Department of Pharmacy and Head of Centre for Advanced Drug Research (CADR) at COMSATS University Islamabad, Abbottabad Campus since 2007. Prof. Iqbal has completed his early education from Pakistan, while he got his MS and PhD degree from University of Strathclyde, Glasgow, UK and University of Bonn, Germany, respectively. After doing 2 Postdocs from Germany and China, he opted to serve Pakistan and joined Department of Pharmacy, COMSATS University, Islamabad, Abbottabad Campus. He has made notable contributions in Pharmaceutical/Chemical Sciences. Prof. Iqbal has more than 270 publications (Impact factor >850) in medicinal chemistry, enzyme kinetics, natural products chemistry, drug discovery and metabolism, molecular modelling and molecular toxicology. In addition to research publications, he has 2 international patents. He has supervised >50 PhD and MS scholars and earned >240 Million PKR research funding from HEC-Pakistan, COMSTECH-TWAS, OPCW, and DAAD-Germany. His scientific and capacity building contributions have been recognized by prestigious national and international awards and honors, and fellowships of several academies of Science and Technologies. According to the RESEARCH PRODUCTIVITY AWARDS (RPA) list issued by Pakistan Council for Science and Technology Prof. Iqbal was awarded “A” category. In 2017, Prof. Iqbal has been awarded PAS-Gold Medal by Pakistan Academy of Sciences. In 2021, the Ministry of Science and Technology and the Ministry of Foreign Affairs, Government of Pakistan, has appointed as a member of Task Force on Science Diplomacy. In addition to his research activities Prof. Iqbal has served the COMSATS University, Islamabad, as a member of Board of Advanced Studies and Research (BASAR), Member of Academic Council, Departmental Advisory Committee, and Convener of Research Productivity Award Committee. Prof. Iqbal has served as editorial board member and reviewer of several international Journals.

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Dr. Wang is a professor of Bioorganic Medicinal Chemistry, Deputy Director of the State Key Laboratory for the Chemistry and Molecular Engineering of Medicinal Resources, School of Chemistry and Pharmaceutical Science, Guangxi Normal University, China. He is also the Chairman of the special primary foundation for the National Key Basic Research Program of China and National Natural Science Foundation of China, and a Member of the Chinese Chemical Society and “Distinguished Experts of Guangxi China”. He got his B.Sc. in Plant Physiology, M. Sc. in Phytochemistry, Doctor's degree (Ph.D.) in Biochemistry, Specialist in polypeptide biochemistry, at the State Key Laboratory of Applied Organic Chemistry, Lanzhou University of China. Dr. Wang got the “Science and technology award of Guangxi” seventh during 2012-2016, respectively. Currently Dr. Heng-Shan Wang’s researches focus on the “Therapeutic Basis of important Medicinal Resources of Guangxi”, “Natural compound derived from traditional Chinese medicine”. Studies on the anticancer mechanisms of apoptotic pathway-targeted natural product-like compound and their derivatives. He published more than 180 papers on *Org. Lett.*, *Green Chem.*, *Chem. Commun.*, *Bioconjugate Chem.*, *J. Med. Chem.*, *Eur. J. Med. Chem.*, *Adv. Synth. Catal.*, *Phytochemistry*, *Phytomedicine*, and *Food Chemistry*, and obtained ten Chinese patent authorizations.

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Prof. Liu was born in Feb. 1977 in Hebei province of China. He received the Bachelor degree of Engineering from Tianjin University (China) in 2000, the Master degree of Engineering from Beijing University of Chemical Technology (China) in 2003, and the Doctorate of Science from Nankai University (China) in 2007. From 2007 till now, he was employed in Guangxi Normal University (China) and engaged in teaching and scientific researching. In 2008, he was moved up to an associate professor and was chosen as a tutor for graduates. Then he finished a post-doctoral program in the following two years. In 2014, he was then moved up to a professorship.

His research interests mainly focused on inorganic medicinal chemistry and bioinorganic chemistry, to develop new metal-based anticancer agents and veterinary drugs. He has published over 50 research papers on SCI-indexed journals, and has been authorized for 25 Chinese invention patents.

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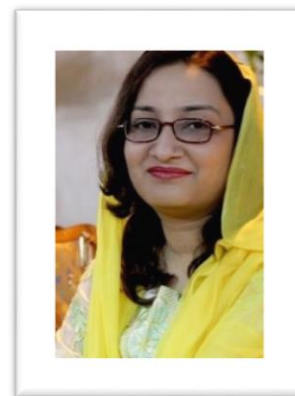
Dr. Reaz Uddin is currently working as an Associate Professor at the PCMD, ICCBS, University of Karachi. His focused area of research is Computational Biology and Bioinformatics. The research is focused on the applications of new computational methods in order to solve medicinal chemistry related problems such as drug discovery against infectious diseases. His particular focus is the resistant microbial pathogens for which the enormous amount of genomics data is available to be analysed by the latest technologies introduced in the areas of Computational Biology and Bioinformatics. He has 55 peer reviewed research articles published in high impact factor international journals.

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Dr. Hina Siddiqui has received her Ph. D. from H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi. During her doctoral studies she went to Department of Chemistry, University of Kansas, USA. She also got postdoctoral training at Department of Chemistry, University of Tübingen, Germany. She has received external funding including industrial funds for establishing and sustaining a good quality research programs. She has published several good papers and submitted patents. Her research interests include discovery of multi-drug resistance reversal agents, drug re-purposing and re-positioning studies, development of new synthetic methodologies for use in drug development and to probe the chemical space through combinatorial libraries. Central to this goal, currently she is working on the synthesis of biologically active heterocyclic compounds. She has also trained several younger scholars at M. Phil. and Ph. D. Level. In addition to this she has trained several foreign students in her laboratory. She has over 35 research publications in peer reviewed high impact factor international journals.