

Curriculum Vitae and Selected Publications
of
Prof. Dr. Zaheer Ul-Haq
Head Computational Medicinal Chemistry Group
FCSP, MACS, AvH Fellow, Fulbright Fellow

*Dr. Panjwani Center for Molecular Medicine and Drug Research,
International Center for Chemical and Biological Sciences,
University of Karachi, Karachi-75270, Pakistan.*

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Personal Data

Full Name : Prof. Zaheer Ul-Haq
Father's Name : Anwar-ul-Haq Qasmi
Date of Birth : January 1ST 1978
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Current Status

Professor

Head Computational and Natural Product Chemistry Group

Dr. Panjwani Center for Molecular Medicine & Drug Research
International Center for Chemical & Biological Sciences
University of Karachi
Karachi-75270, Pakistan
www.iccs.edu

Research Interest

- Design of new bio-active molecules using computer aided modelling techniques
- Modelling of small organic molecules, proteins, and protein-ligand interactions
- Ligand based and structure based pharmacophore design
- Generation and screening of large virtual combinatorial compound libraries
- Molecular activity determination using 3D-QSAR or quantum chemistry calculations
- Molecular Dynamics (MD) simulations studies of protein-ligand complex
- Computational chemistry of natural products

ACADEMICS

- 2006 Fulbright Fellow** : Advisor Prof. Jeffery Madura, Duquesne University, USA
- 2003 Postdoctoral Fellow** : Advisor Prof. Dr. DDD. h.r. Bernd Michael Rode, University of Innsbruck, Innsbruck, Austria.
- 2002 Ph. D. (Chemistry)** : Advisor Prof. Dr. Atta-ur-Rahman, University of Karachi, Pakistan.
- 1999 M. Phil / Ph. D. courses** : HEJ Research Institute of Chemistry, University of Karachi, Pakistan.
- 1998 M.Sc. (Organic Chemistry)** : University of Karachi, Pakistan.
- 1996 B.Sc. (Hons.) (Chemistry, Bio and Physio)** : University of Karachi, Pakistan.

Experience:

Professor (Tenured) : (June 2020 to Present)

Head Computational Medicinal Chemistry Group,
Dr. Panjwani Center for Molecular Medicine, ICCBS, University of Karachi, Pakistan.

Associate Professor : (Jan 2016 – June 2020)

Head Computational Medicinal Chemistry Group,
Dr. Panjwani Center for Molecular Medicine, ICCBS, University of Karachi, Pakistan.

Visiting Scientist : (April 2018 – August 2018)

Department of Bio-Molecular Sciences,
University of Mississippi, Mississippi, USA

Alexander von Humboldt Fellow : (May 2013- Dec-2013)

Heidelberg Institute for Theoretical Studies,
Heidelberg, Germany

Visiting Professor : (Jan 2012 – Dec-2019)

Atta-ur-Rahman School of Applied Biosciences,
National University of Science and Technology, Islamabad, Pakistan.

Alexander von Humboldt Fellow : (Oct 2010- Jan 2012)

Heidelberg Institute for Theoretical Studies,
Heidelberg, Germany

Visiting Scientist : (Jan 2010 - Feb 2010)

Computational Inorganic Chemistry Group; Inorganic Chemistry Laboratory, University of Oxford, UK

Visiting Scientist : (Dec 2008 - Jan 2009)

[Department of Theoretical Chemistry](#), Institute of General, Inorganic and Theoretical Chemistry,
University of Innsbruck, Innrain 52a, A-6020 Innsbruck, AUSTRIA

Assistant Professor : (March 2007 – Dec 2015)

[Dr. Panjwani Center for Molecular Medicine](#), ICCBS,
University of Karachi, Pakistan

Senior Fulbright Fellow : (Sep 2006 – Jun 2007)

[Advisor Prof. Jeffrey D. Madura](#), Department of Chemistry & Biochemistry,
Center for Computational Sciences, Duquesne University, Pittsburgh, PA

eCheminfo Advanced Training : (July 3-7, 2006)

Latest Advances in Drug Discovery Design & Planning Methods,
Chemistry Research Laboratory, Oxford University, Oxford, UK.

Visiting Scholar : (13th – 21st June, 2005)

Pharmaceutical Biosciences, Division of Pharmaceutical Pharmacology,
Uppsala University, Sweden

Research Associate : (2001-2002)

PSF-S-Ku/Chem Project, HEJ Research Institute of Chemistry,
University of Karachi, Pakistan.

Scholarship and Awards:

➤ CSP Gold Medal for Chemist under 40	2016
➤ Cash Award of Research Productivity Allowance (RPA)	2010-17
➤ Selected to participate in the 61 st Lindau Meeting of Nobel Laureates	2011
➤ Alexander Von Humboldt - Georg Forster Research Fellowship	2010
➤ INSPIRE for the Talented Researcher Exchange Award	2009
➤ Prof. Atta-ur-Rahman Gold Medal in Chemistry	2008
➤ Award of "Star Laureate 2007" by South Asia Publication	2008
➤ Cash Award of Research Productivity Allowance (RPA)	2007
➤ Occasional Lecture Program (OLP) Award	2007
➤ Senior Fulbright Scholarship	2006
➤ Cash Award of Research Productivity Allowance (RPA).	2004-2005
➤ IBRO Fellowship on Cholinesterase (Italy)	2004
➤ Austrian Postdoctoral Fellow Ship	2002
➤ First Prize for Best Poster in 7 th EuroAsia Conference	2002
➤ Fellowship of H.E.J. Research Institute of Chemistry	1997 – 2002
➤ Vice-chancellor scholarship	1997
➤ Vice-chancellor scholarship	1996
➤ President cum talent scholarship	1995

Proficiencies:

- Relevant Skills: Molecular Modeling, Drug Design, Virtual Screening, Docking,
- Molecular Dynamics, Computational Chemistry, Cluster Analysis, Drug Discovery.
- Software of relevance in Computational Medicinal Chemistry: ICM, Modeller, AMBER, NAMD, ACEMD, G09, enhanced sampling tools (PLUMED), Schrodinger (MCPRO+, LigPrep, MacroModel).
- OSs and Programming Languages: Linux, MacOS, and Windows; Matlab, Python.
- Preliminary understanding of computational chemistry theory, and very proficient in the operation of most computational chemistry software.
- Detailed knowledge of computers operating system including UNIX, Linux, Macintosh and Windows, Installation, maintenance and repairing.
- Experience in Medicinal Chemistry packages including Amber, Sybyl, Autodock, Rasmol, Molmol, FlexX, Gaussian, GaussView, Molden, CS Chem Office, software compilation, desktop publishing, and hardware assembly.
- Detailed knowledge of almost all organic laboratory equipment, especially NMR (including 19F-NMR, 2D-NMR, and chiral shift reagents), FT-IR, GC, GC-MS, LC-MS, HPLC (analytical and prep), chromatography, photochemical apparatus, low temperatures, inert atmospheres.
- Isolation, degradation, and derivatisation of natural products. Structure elucidation with modern NMR techniques including acquisition of 2D NOE and inverse detected experiments. Use of current analytical and predictive tools including HPLC, GCMS, LCMS and Counter current chromatography.
- Proficient with the operation, maintenance, and small repairs of technical and sensitive lab equipment (HPLC pumps, rotary chromatotrons, vacuum apparatus)
- Success as a laboratory and tutorial instructor in general and organic chemistry. Experienced working in a multidisciplinary team. Appropriate organization, record keeping, verbal and written communication skills.
- Urdu (native), English (Fluent), German (Basic)

International Editorial Board Member:

Journal of Molecular Graphic and Modeling since 2011

Current Computer-Aided Drug Design since 2016

The Natural Product Journal since 2019

Manuscript Reviewer:

Journal of Medicinal Chemistry

Journal of Chemical Information and Computer Sciences

Journal of Bio-organic and Medicinal Chemistry Letters

Egyptian Pharmaceutical Journal

Journal of Molecular Modeling

Journal of Enzyme Inhibition and Medicinal Chemistry

Chemical Biology & Drug Design

Journal of Molecular Structure

Conferences/Workshops Organized:

Organized Workshop on Bioinformatics, Riphah International University, Islamabad, March 13-14, 2019.

Organized Workshop on Computational Chemistry: 1st National Workshop on Computational Chemistry and Drug Designing, Department of Chemistry, U.S.T Bannu, KPK, December 19-20, 2018.

Organized Workshop on Bioinformatics, Riphah International University, Islamabad, November 15-16, 2017.

Organized Workshop on Computational Chemistry: A New Approach to Understanding & Solving Chemical Problems, Department of Chemistry, Forman Christian College, Lahore, Jan 20- 22, 2016.

Organized Workshop on Computational Chemistry and Drug Design at the International Bhurban Conference on Applied Sciences & Technology (IBCAST), National Centre for Physics (NCP), Islamabad, Jan 12-16, 2016.

Organized NASIC Conference Cum Workshop on Herbal Drug Development for Socio-Economic Uplift in Developing World, University of Jordan, Amman- Jordan, Sep 6-8, 2015.

Mini Workshop on 5th International Symposium-Cum-Training Course on Molecular Medicine and Drug Research (MMDR-5) on Finding Lead Molecules through Computational Techniques, ICCBS, PCMD, University of Karachi, Karachi, Jan 12-15, 2015.

Organized 1st International Workshop on Computer-Aided Drug Design, Department of Chemistry, University of Jordan, April 23-25, 2013.

Organized National Symposium on Computational Biology in Pakistan "Current Status and Future Challenges" COMSATS Institute of Information Technology, Islamabad, November 8-9, 2012.

Organized Workshop on Bioinformatics in Medicine, Institute of Basic Medical Sciences, Khyber Medical University, Peshawar, May 14-15, 2012.

Organized 13th International Symposium on Natural Products Chemistry (ISNPC-13), held in Karachi, September 22 – 25, 2012.

Organized Sustainable and Collaborative Research Networks, ICCBS, Karachi under British Council, UK, December 3-4, 2010.

Organized "11th International Symposium on Natural Product Chemistry" held in Karachi, October 29th to November 1st, 2008.

Organized "1st International Workshop-cum-Training Course on Molecular Medicine and Drug Research" PCMD, Karachi, January 16 - 30, 2007.

Organized "National Workshop on Computational Chemistry and Its Applications", Karachi, Pakistan, June 26-28, 2006.

Participation in Conferences/Workshops:

- Guest Speaker in the “Drug and Vaccine Design in the Era of Pandemic Satellite Virtual Symposium in conjunction with the INTERNATIONAL CONFERENCE ON DRUG DISCOVERY AND TRANSLATIONAL MEDICINE 2021 (ICDDTM’21)” Organized by Malaysian Association for Cancer Research, Malaysia, November 17, 2020.
- Invited Lecture in “3rd International Conference on Recent Innovations in Pharmaceutical Sciences” organized by Riphah International University, Islamabad, March 13-14, 2019.
- Invited Lecture in “1st International Conference on Medicinal Chemistry & Drug Discovery” organized by COMSTECH Islamabad, October 18 – 19, 2018.
- The 5th Annual Drug Discovery and Development Colloquium, University of Kentucky, **Lexington, KY**, June 21-23, 2018.
- The 45th Annual MALTO Medicinal Chemistry-Pharmacognosy Meeting-in-Miniature, at Texas A&M University, College Station, **Texas**, May 23-25, 2018.
- Invited Lecture in “2nd International Conference on Recent Innovations in Pharmaceutical Sciences” organized by Riphah International University, Islamabad, November 15-16, 2017.
- Keynote lecturer in “Hands-on Workshop and Humboldt-Kolleg: Density-Functional Theory and Beyond - Basic Principles and Modern Insights” Organized by Isfahan University of Technology Isfahan, **Iran**, May 2 - 13, 2016.
- Invited Lecture in “Symposium on Recent Trends in Chemical Sciences” Organized by Federal Urdu University of Arts, Science and Technology, **Urdu University** of Arts, Science and Technology, April 12, 2016.
- Invited Lecture on “Protein modeling” at Department of Biosciences, **SZABIST**, Karachi, January 28, 2016.
- Invited lecture in the 1st International Conference on Drug Discovery and Development, Organized by International Center for Genetic Engineering and Biotechnology, Dhaka, **Bangladesh**, October 3-6, 2015
- Invited Lecture in the 1st International Conference on Natural Products & Drug Discovery, Organized by The University of Jordan, Amman- **Jordan**, Sept 8-10, 2015.
- Invited Lecture in “2nd International Conference on Drug Development Natural & Synthetic at COMSATS Institute of Information Technology, **Abbottabad**, Aug 23 - 25, 2015.
- ACSE Annual Meeting Short Course for Journal Editors on “Marketing for Scholarly Journals, Developing A Successful Journal, Publication, Ethics, Peer Review and Metrics”, Organized by Asian Council of Science Editors held in Dubai, **UAE**, Aug 13-14, 2015.
- Participated in National Seminar on “Chemical Safety and Security Management and Role of Stakeholders”, Organized by National Authority of Chemical Weapons Convention of Islamic Republic of Pakistan, 15 June 2015.
- One Day Session on “Internal Compliance Procedures” Office of Research, Innovation & Commercialization (ORIC), NED University of Engineering and Technology, June 12, 2015.
- Participated in Workshop On “How to Give an Effective Lecture?” at PCMD, ICCBS, University of Karachi. Jointly Organized by PCMD and VEPP, May 27, 2015.
- Meeting of Experts for “Establishing an Advance Computational Facility in COMSTECH” Organized by COMSTECH OIC (Organization of Islamic Cooperation), April 27, 2015.
- Invited Lecture in “1st International Conference on Recent Innovations in Pharmaceutical Sciences” at Riphah University of Pharmaceutical Sciences, March 3-5, 2015.
- Participated in the Workshop on Intellectual Property Rights Management Through Patents Organized by ICCBS, University of Karachi, Karachi. Pakistan, Jan 8-9, 2015.
- Participated in the Workshop on Scientific Writing Organized by ICCBS, University of Karachi, Karachi, Jan 5 - 7, 2015.

- Participated in the Workshop On “Modern Spectroscopic Techniques and Their Applications in Structure Determination” Organized by ICCBS, University of Karachi, Karachi under the Auspices of Network of Academies of Sciences in Islamic Countries (NASIC) Dec 1 - 3, 2014.
- Invited Lecture in “Foundation for Integrated Sciences, Posters Exhibition On “Small Variations for Big Changes” & Workshop On “Bioinformatics”: Tools & Techniques in Modern Research” at DIMC, DUHS, Karachi, Nov 7-8, 2014.
- Presentation in “25th National and 13th International Chemistry Conference, A Silver Jubilee Event of The Chemical Society of Pakistan” held at Institute of Chemistry, University of The Punjab, Lahore, Pakistan, October 20 – 22, 2014.
- Guest Speaker On Bioinformatics Series of Lectures “Bioinformatics; As Emerging Science and Its Future” Organized by The Aligarh Institute of Technology (AIT), Sep 4th, 2014.
- Deliver presentation in “Emerging Trends in Bioinformatics and Computational Biology” held in Mohammad Ali Jinnah University, Islamabad, June 7th, 2014.
- Invited Lecture in “A Journey from Natural Product Chemistry to Computational Medicinal Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, UK, Feb 10, 2010
- Participated in “6th International Symposium of the Austrian Proteomics Platform” held in Seefeld, Austria, January 18-21, 2009.
- Presentation in “11th International Symposium on Natural Product Chemistry” held in the ICCBS, Karachi, October 29th to November 1st, 2008.
- Invited Lecture in “1st Junior National Chemistry Conference under the age of 35” Department of Chemistry, Muzaffarabad, October 19-22, 2008.
- Presentation in “International Workshop on Biotechnology for Development” held in Kohat University of Science and Technology, Kohat, March 4-5, 2008.
- Deliver presentation in “The 18th National Chemistry Conference” held in The Punjab University, Lahore, February 25-27, 2008.
- Deliver presentation in “233rd ACS National Meeting” held in Chicago, USA, March 25-29, 2007.
- Invited lecture entitled “Lead Discovery through Combination of Natural Product and Computational Chemistry” at Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois at Chicago, Chicago, USA, March 26th, 2007.
- Invited lecture entitled “A Computational Approach for Exploiting Bioactive Natural Product” at Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, USA, March 16th, 2007.
- Delivered lecture in “20th "Darmstadt" Molecular Modeling Workshop” Computer-Chemie-Centrum, Erlangen, Germany, May 23 – 24, 2006.
- Invited lecture entitled “Computational Chemistry for Beginner” at Chemistry Department, Jinnah University for Women, Karachi, August 2nd, 2006.
- Deliver presentation in “The 6th International & 16th National Chemistry Conference” held in Bahauddin Zakariya University, Multan, April 6-8, 2006
- Invited lecture entitled “The Role of Computational Chemistry in the Process of Drug Discovery” at Chemistry Department, Quaid-e-Azam University, Islamabad, March 22nd, 2006.
- Delivered lecture in “The 10th International Symposium on Natural Product Chemistry, Karachi, Pakistan, January 06-09, 2006.
- Invited lecture entitled “Structure-Based Drug Design using 3D-QSAR and Molecular Docking Techniques” at Pharmaceutical Biosciences, Division of Pharmaceutical Pharmacology, Uppsala University, Uppsala, Sweden, June 14th, 2005.
- Invited lecture entitled “Application of 3D-QSAR and Molecular Docking Technique” at Computer Aided Molecular Design Group, Department of Pharmaceutical Chemistry, University of Innsbruck, Innsbruck, Austria, June 23rd, 2005.

- Delivered presentation in “The second international conference of pharmaceutical and drug industries division” National Research Centre (NRC), Cairo, Egypt, March 7-9, 2005.
- Delivered presentation in “8th International Symposium on Protein Structure Function Relationship. Jan. 7-10, 2005.
- Deliver presentation in the 5th International and 15th National Chemistry Conference at Islamabad, 24th to 27th of Nov 2004
- Participated in the 9th International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 10-13, 2004.
- Presented poster in the 7th Euroasia Conference on Chemical Sciences, Karachi, Pakistan, March 9-12, 2002.
- Participated in the 8th International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 18-22, 2000.
- Participated in the 6th International Symposium on Protein Structure-Function Relationship, Karachi, Pakistan, Feb. 5-7, 1999.
- Presented poster in the 9th National Chemistry Conference, Karachi, Pakistan, Dec. 4-6, 1998.
- Participated in the 7th International Symposium on Natural Product Chemistry, Karachi, Pakistan, from Dec. 28, 1997 to Jan. 1, 1998.

TEACHING-Activities

Deliver lectures to MPhil and PhD students on various aspects of Chemistry, Bio-Chemistry, such as Spectroscopy, Natural Product Chemistry, Proteomics, Bioinformatics, Computational Biology.

Courses designed for PhD students

- (1) Structural Biology
- (2) Protein Chemistry

Deliver lectures in the following MPhil/PhD courses at HEJ, ICCBS

- Computational Biology (MM-707)
- Analysis of Structure-Activity Relationships
- Bioinformatics and Protein Modelling (MM-701)
- Molecular Modelling for Pharmacists
- Rational Drug Design (653)
- Pharmacoinformatics (Seminar)
- Laboratory Course – Drug Analysis and –development (including *in silico* methods)
- General Spectroscopy, including 1 and 2D NMR, UV-IR, Mass Spectroscopy
- General Organic Chemistry
- Reaction Mechanism
- Reaction Catalysis (CHEM-742)

M. Phil/Ph. D. Thesis Supervised:

Name	Title	Degree	Year
32) Javaria Ashraf	Formal Modeling and Analysis of The Amyloidogenic Pathway in Alzheimer's Disease	Ph. D.	2020
31) Juweria Effendi	<i>In-silico</i> based modeling of Interleukin-2 Induced T-Cell Kinase inhibitors.	Ph. D.	2020
30) Ruqaiya Khalil	Implementation of Cheminformatic Approaches to Identify Protozoan Protein Acylation Inhibitors	Ph. D.	2019
29) Sehrish Naz	Tailoring Anti-inflammatory Cytokine Inhibitors: A Fragnomics Approach.	Ph. D.	2019
28) Rabia Iqtadar	In-silico experimental correlation of degradation products of antipsychotic drugs: Fluvoxamine & Risperidone. (Co-Supervisor)	M. Phil	2019
27) Sobia Iftakhar	Photo Biological and Photochemical Behavior of Photosensitive Anti-Diabetic Drugs: Metformin and Rosiglitazone. (Co-Supervisor)	M. Phil	2019
26) Sajjad Haider	Identification of Novel Inhibitors for Cxcl12 Through Computational Techniques	M. Phil.	2019
25) Komal Zia	In Silico Identification of Potent Inhibitors Against Tumor Necrosis Factor Alpha (TNF- α)	M. Phil.	2019
24) Lubna Atta	Computational Approaches to Develop Therapeutic Agents Against Cariogenic Biofilms.	M. Phil.	2019
23) Sajda Ashraf	Computer Aided Drug Design and Analysis of Protein Kinases and Other Related Targets.	Ph. D.	2018
22) Munneeb Ali	Designing of Novel Insulinotropic Molecules for key targets in Insulin Secretion Through Computational Techniques.	M. Phil.	2018
21) Alamgir Khan	Theoretical Studies on Assorted IKK β and its Inhibitors.	M. Phil.	2018
20) Bakhtawer Qurashi	Theoretical Studies on Thymidylate Kinase and Its Inhibitors	M. Phil.	2018
19) Urooj Qurashi	Identification of novel isoform-selective antagonist of Exchange Protein Activated by c-AMP 2	M. Phil.	2018
18) Abid Channa	Molecular Dynamics Simulations of Biologically Important Proteins.	M. Phil.	2017
17) Tahir Ayub	Computational Studies on Diverse Ikk β Inhibitors	M. Phil.	2016

16) Uzma Mahmood	Identification of Novel Cholinesterase and Other Biological Target Inhibitors Using Computer Aided Drug Design Strategy (Co-Supervisor).	Ph. D.	2016
15) Mariya Yousuf	Computer Aided Studies of Potent α -Chymotrypsin and β -Glucuronidase Inhibitors	Ph. D.	2016
14) Naveed Khan	<i>In Silico</i> Characterization of Inhibitors Against Lipoxygenase and other Medicinally Relevant Enzymes	M. Phil.	2015
13) Sana Gul	Computer Aided Drug Design Strategies to Model Thymidine Monophosphate and other Related Kinase Inhibitors	Ph. D.	2015
12) Kashif Zafar	Molecular Dynamics Simulation Study of Pulmonary Surfactant Interacting with Nanoparticles	M. Phil.	2014
11) Saman Usmani	Theoretical Studies on Immuno-modulatory Protein	M. Phil.	2013
10) Waqas U. Khan	Understanding Protein-Ligand Interactions Involved in Immune Activation and Other Therapeutic Charges	Ph. D.	2013
9) Huma Naseem	Computer Based Drug Design, Synthesis and Analgesic Evaluation of Some Nitrogen Containing Heterocyclic Compounds (Co-Supervisor).		
8) Rehana Zia	Molecular Dynamics Simulation and Binding Free Energy Calculation on InterLeukin-2 and its Complex	M. Phil	2013
7) Sobia A. Halim	Modeling Aided Lead Design of Cytokines Inhibitors	Ph. D.	2013
6) Sadaf Iqbal	Theoretical and Experimental Structure-Function Studies on Medicinally Important Proteins	Ph. D.	2012
5) Tarique Moin	Molecular Dynamics Simulations of Lipoxigenase and Other Hydrated Molecules by Force Field and Quantum Mechanical Method	Ph. D.	2012
4) Abdul Wadood	Computer-Aided Development of New Urease Inhibitors.	Ph. D.	2010
3) Riaz-ud-Din	Computational Studies of Cholinesterase Inhibitors and Biological Studies of Related Enzyme.	Ph. D.	2009
2) S. Lal Badshah	Molecular Dynamics Simulation of Cholera Toxin A-1 Polypeptide (Co-Supervisor)	M. Phil.	2009
1) Uzma Mahmood	Structural and Molecular Modeling Studies on Cholinesterase Inhibitors	M. Phil.	2009

Students Enrolled in M. Phil/PhD: Currently following students are enrolled in M. S. / Ph. D. under my supervision.

No.	Name	Title
1)	Hina Qaiser	Computer Aided Drug Design Strategies (CADD) to Model Inflammatory Cytokine Inhibitors as Drug Target in Autoimmune Disorders.
2)	Saman Yousuf	Molecular Dynamics Simulation of Proteins that Involved in Folate Pathway.
3)	Alamgir Khan	Theoretical Analysis of Covalent Complementarity of Tyrosine Kinases and other Related Targets.
4)	Urooj Qureshi	Unrevealing the Structural Insights of EPAC Along with its Variants and other Related Targets
5)	Bakhtawar Qureshi	Ensemble Based Generation of New Antagonist of IPMK and other Related Targets
6)	Komal Zia	<i>In silico</i> Identification of Potent Inhibitors against Tumor Necrosis Factor Alpha (TNF- α).
7)	Lubna Atta	Computational Approaches to Develop Therapeutic Agents Against Cariogenic Biofilms
8)	Sajjad Haider	Identification of Novel Inhibitors for CXCL12 Through Computational Techniques
9)	Nizakat Ali	Molecular Dynamics Simulation Study to Explore the Rev Response Element RNA of HIV-1.
10)	Mehar Sanam	Computational Studies on The Addictiveness Profile of Recreational and Plant-Based Drugs of Abuse
11)	Zaid Anis	Designing of Negative Allosteric Modulators of NMDA Receptors Targeting GluN2A Subunit through Computational Techniques
12)	Sonia	Theoretical Studies for the Possible Role of Glycoproteins in Memory
13)	Mamona Mushtaq	Design of New Small Molecule Inhibitors Targeting Dengue Virus Protease: An <i>In silico</i> Approach.
14)	Madiha Sardar	Targeting Anti-inflammatory Drugs for Potential Antidepressant Activity
15)	Salman Ali	Functional Characterization of Galanin Receptor and its Subtypes
16)	Maria Mushtaq	Structural Characterizations and Selective Inhibition of Bromodomain Containing Proteins
17)	Syada Mahpara (Co- Supervisor)	In Preparation
18)	Israr Khan	Exploring the Insulin Secretory Mechanism of Eupatorin and

- (Co- Supervisor) Hymercromone In Pancreatic Islets of Langerhans
19) Dure Shahwar Targeting microvascular α 2C-adrenoceptor protein-protein
(Co-Supervisor) interaction using *in-silico* and experimental approaches
20) Shakeeb In Preparation
(Co- Supervisor)
22) Fariha Naz Modulation of Insulin Secretory Pathways by Potent Insulin Secretagogue
(Co- Supervisor) in Mice Islets

Master Thesis Supervised:

Name	Title	Year
Hasnain Tariq	In Silico Analysis of Thymidylate Inhibitors of S. Aureus Thymidylate Kinase	2016-17
Irum Mehboob	Identification of EPAC2 Antagonist; Pharmacophore Based Virtual Screening	2016-17
Sana Gul	Structure Based Lead Identification of Thymidine Mono-phosphate Kinase Inhibitors as Antitubercular Agents	2009-10
Sauleha Khan	Virtual Screening of Cytokine Inhibitors: Application of Docking & Pharmacophore Models	2009-10
Sonia Jokhio	Molecular and Structural Analysis of Adamantyl Susceptibility to HLA-RSs Allelic Variants	2009-10
Bushra Taj	Comprehensive Structural Elucidation & Insight into Potential Interaction of Rat NEP2 Protein with Inhibitors of Varying Potency Revealing Functional Diversification	2009-10
Amal Jalil	Virtual Screening of Novel Non-Nucleoside HIV-1 Reverse Transcriptase	2008-09
Saqib Faisal	Study of Protein-Ligand Interaction by Computational Chemistry Tools.	2007-08
Bushra Jahangir	Structure Based 3D-QSAR Studies on Physostigmine Derivatives as Cholinesterase Inhibitors	2007-08
Lina Asif	3D-QSAR and Molecular Docking Studies of Podophyllotoxin Analogues as Tubulin Inhibitor	2006-07
Mehwish Aleem	Understanding the Antitumor Activity of Acylsulphonamide Derivatives Using Molecular Docking and 3D-QSAR Studies	2006-07
Erum Gul	Molecular Docking Studies of Urease Inhibitors	2005-04
Sobia Halim	Different Docking Approach to Explore Protein-Ligand Interactions	2005-04
Mehrin Khan	Theoretical Analysis of The Active Site of Cholinesterase Enzyme.	2005-04

Research Grant Awarded as PI:

No	Title of Project	Amount	Funding Agency	Year
1)	Molecular Dynamics Simulation of Nanoparticles	Euro 18,500	Alexander von Humboldt	2017
2)	Computer Guided Synthesis and Biological Evaluation of Novel Immuno-modulatory Agents.	US \$ 8,900	COMSTECH-TWAS, Trieste, Italy	2016
3)	Upgradation of Scientific Equipment	Rs.943,000	HEC, Pakistan	2016
4)	Theoretical and Computational Studies of Zinc Metalloproteinases.	Rs 2,503,080	HEC, Pakistan	2011
5)	Structure-Based Approach to Design Antiparasitics: Inhibition of Folate Pathway Enzyme in Leishmania and Trypanosoma.	Rs 2,651,694	Higher Education Commission, Pakistan	2010
6)	Structure-based Drug Design to Identify New Lipoxygenase Inhibitors and to Explore their Binding Mechanism	Rs 2,652,360	Higher Education Commission, Pakistan	2010
7)	Computer aided Identification of Cholinesterase Inhibitors for the Treatment of Alzheimer's Disease and Related Dementia.	Rs 1,174,860	Pakistan Science Foundation, Pakistan	2010
8)	Workshop on Building Sustainable Research Networks	Rs 183,000	British Council, UK	2010
9)	Austrian-Pakistan Cooperation Project in Computational Chemistry		Austria	2010
10)	INSPIRE for the Talented Researcher Exchange Programme.	Rs. 230,000	British Council, UK.	2009
11)	Collaboration with the Theoretical Chemistry Department, University of Innsbruck, Austria in the Field of Computational Chemistry Research.	Rs. 184,800	Higher Education Commission, Pakistan	2009
12)	Strengthening and Up gradation of Computer-Aided Drug Design Laboratory at the Dr. Panjwani Center for Molecular Medicine and Drug Research.	Rs. 915,702	Higher Education Commission, Pakistan	2007
13)	An <i>In Silico</i> Approach to Discovering Novel Inhibitors for Helicobacter Pylori Urease: A Valid Target for Anti-Ulcer Therapy.	Rs 2,762,160	Higher Education Commission, Pakistan	2005
14)	Research Grants to Active Scientists/Technologists of Pakistan	Rs. 990,000	Pakistan Science Foundation	2005
15)	Collaboration with the Pharmaceutical Biosciences, Pharmacology Department, Uppsala University in the Field of Proteo-Chemometrics Research.	Rs. 299,400	Higher Education Commission, Pakistan	2005
16)	Start-up Funds from Dr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical Sciences.	Rs.10,00,000	University of Karachi	2004

Research Grant Awarded As Co-PI				
17)				
18)	Microvascular α_2 C-adreno receptors: Targeting protein-protein interaction for treatment of peripheral vascular disease.	Rs. 16,927,585	HEC, Pakistan	2017
19)	Identification of Herbal Medicine as A Potential Xanthine Oxidase Inhibitors by Using Virtual Screening.	Rs 1,995,640	HEC, Pakistan	2016
20)	Understanding Molecular Basis of Anti-myloidogenic Properties of EGCG	Rs 500,000	HEC, Pakistan	2015
21)	Computer-guided Design and Synthesis of IL2 Inhibitors as Immunomodulating Agents.	Rs 4,820,000	HEC, Pakistan	2010
22)	Studies towards rationally designed molecules of biological interests using natural products as models.	Rs 4,280,000	HEC, Pakistan	2010



Zaheer UL-HAQ

Professor

Dr. Panjwani Center for Molecular Medicine

[Computational Chemistry](#), [Drug Design](#)

[Biophysics](#)

Google Scholar

	All	Since2016
Citations	2775	1688
h-index	28	19
i10-index	74	56

Books / Chapters

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