

**Curriculum Vitae and Selected Publications**  
**of**  
**Dr. Zaheer ul-Haq**  
*Assistant Professor*

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*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 : Dr. Zaheer-ul-Haq  
Father's Name : Anwar-ul-Haq Qasmi  
Date of Birth : January 1<sup>ST</sup> 1978  
Permanent Address : E-75, Alflah Malir Halt,  
Karachi-75210, Pakistan.  
E-mail Addresses : [zaheer.qasmi@iccs.edu](mailto:zaheer.qasmi@iccs.edu)  
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## **Current Status**

### *Assistant Professor*

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

## **Academics**

### **Postdoctoral Fellow**

**2002-2003**

Advisor Prof. Dr. DDD. h. r. Bernd Michael Rode  
University of Innsbruck, Innsbruck, Austria.  
(MD Simulation, Docking, Modelling and QSAR studies)

### **Ph. D. (Chemistry)**

**1998- 2002**

Advisor Prof. Dr. Atta-ur-Rahman  
Minister of Science and Technology,  
Director H.E.J. Research Institute of Chemistry, University of Karachi.  
(Isolation, Purification and Structural Elucidation of Bio-active Natural Products)

**M.Phil/Ph.D** courses at HEJ University of Karachi **1998-1999**

**M.Sc. (Organic Chemistry)** **1996-1998**  
University of Karachi, Pakistan.

**B.Sc. (Hons.) (Chemistry, Biochemistry and Physiology)** **1993-1996**  
University of Karachi, Pakistan.

### **Experience:**

**Assistant Professor** **March 2004 - till present**  
Dr. Panjwani Center for Molecular Medicine and Drug Research,  
ICCBS, University of Karachi.  
<http://www.iccs.edu>

**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

**Senior Fulbright Fellow** **Sep 06 – Jun 07**  
Advisor Prof. Jeffrey D. Madura  
Department of Chemistry & Biochemistry  
Center for Computational Sciences  
Duquesne University  
[www.duq.edu](http://www.duq.edu)

**eCheminfo Advanced Training** **July 3-7 2006**  
Latest Advances in Drug Discovery Design & Planning Methods  
Chemistry Research Laboratory  
Oxford University, Oxford, UK.

**Visiting Scientist** **May 2006 -June 2006**  
Institute of Pharmacy, Department of Pharmaceutical Chemistry  
Leopold-Franzens-University Innsbruck  
Josef-Moeller-Haus, Innrain 52c, 6020 Innsbruck, AUSTRIA

**Visiting Scholar** **May 2005 -July 2005**  
Institute of Pharmacy, Department of Pharmaceutical Chemistry  
Leopold-Franzens-University Innsbruck  
Josef-Moeller-Haus, Innrain 52c, 6020 Innsbruck, AUSTRIA

**Visiting Scholar** **13<sup>th</sup> – 21<sup>st</sup> June, 2005**  
Pharmaceutical Biosciences,

Division of Pharmaceutical Pharmacology,  
Uppsala University, Uppsala, Sweden  
Contact Person: Prof. Jarl ES Wikberg  
<http://www.farmbio.uu.se/researchgroup.php?fg=1>

**Senior Research Officer** **2003-2004**  
H.E.J. Research Institute of Chemistry,  
University of Karachi.

**Postdoctoral Fellow** **2002-2003**  
Advisor Prof. Dr. DDD. Bernd Michael Rode  
University of Innsbruck, Innsbruck, Austria.  
(MD Simulation, Docking, Modelling and QSAR studies)  
<http://www.uibk.ac.at>

**Research Associate:** **2001-2002**  
Pakistan Science Foundation PSF-S-Ku/Chem Project  
Principle Investigator Dr. Ahsana Dar  
HEJ Research Institute of Chemistry

### **Scholarship and Awards:**

- 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 Lectrue Program (OLP) Award **2007**
- Senior Fulbright Scholarship **2006**
- Cash Award of Research Productivity allowance (RPA) **2005**
- Cash Award of Research Productivity allowance (RPA). **2004**
- IBRO Fellowship on Cholinesterase (Italy) **2004**
- Austrian Postdoctoral Fellow Ship **2002**
- First Prize for Best Poster in 7<sup>th</sup> EuroAsia Conference **2002**
- Fellowship of H.E.J. **1997 - 2002**
- Vice-chancellor scholarship **1997**
- Vice-chancellor scholarship **1996**
- President cum talent scholarship **1995**

### **Proficiencies:**

- 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. All major word processing, presentation, and database manipulation software packages.
- 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 <sup>19</sup>F-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.

### **Manuscript Reviewer:**

[Journal of Medicinal Chemistry](#)

[Journal of Chemical Information and Computer Sciences](#)

[Journal of Bio-organic and Medicinal Chemistry Letters](#)

[Egyptian Pharmaceutical Journal](#)

### **Participation in Conferences/Workshops:**

- Participated in “6<sup>th</sup> International Symposium of the Austrian Proteomics Platform” held in Seefeld, Austria, from January 18-21, 2009.
- Organized and deliver presentation in “11<sup>th</sup> International Symposium on Natural Product Chemistry” held in the ICCBS, Karachi, from October 29<sup>th</sup> to November 1<sup>st</sup>, 2008.
- Participated and deliver Invited Lecture in “1<sup>st</sup> Junior National Chemistry Conference under the age of 35” Department of Chemistry, Muzaffarabad, from October 19-22, 2008.

- Participated and deliver presentation in “International Workshop on Biotechnology for Development” held in Kohat University of Science and Technology, Kohat, from March 4-5, 2008.
- Participated and deliver presentation in “The 18<sup>th</sup> National Chemistry Conference” held in The Punjab University, Lahore from February 25-27, 2008.
- Participated and deliver presentation in “233rd ACS National Meeting” held in Chicago, USA, from 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 26<sup>th</sup>, 2007.
- Invited lecture entitled “A Computational Approach for Exploiting Bioactive Natural Product” at Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, USA, March 16<sup>th</sup>, 2007.
- Participated and 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 2<sup>nd</sup>, 2006.
- Participated and deliver presentation in “The 6<sup>th</sup> International & 16<sup>th</sup> National Chemistry Conference” held in Bahauddin Zakariya University, Multan from 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 22<sup>nd</sup>, 2006.
- Participated and delivered lecture in “The 10<sup>th</sup> 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.
- Participated and delivered presentation in “The second international conference of pharmaceutical and drug industries division” National Research Centre (NRC), Cairo, Egypt, March 7-9, 2005.
- Participated and delivered presentation in “8th International Symposium on Protein Structure Function Relationship. Jan. 7-10, 2005.

- Participated and deliver presentation in the 5<sup>th</sup> International and 15<sup>th</sup> National Chemistry Conference at Islamabad from 24<sup>th</sup> to 27<sup>th</sup> of Nov 2004
- Participated in the 9<sup>th</sup> International Symposium on Natural Product Chemistry, Karachi, Pakistan, January 10-13, 2004.
- Participated in the 7<sup>th</sup> Euroasia Conference on Chemical Sciences, Karachi, Pakistan, March 9-12, 2002.
- Participated in the 8<sup>th</sup> International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 18-22, 2000.
- Participated in the 6<sup>th</sup> International Symposium on Protein Structure-Function Relationship, Karachi, Pakistan, Feb. 5-7, 1999.
- Participated and presented lecture and poster in the 9<sup>th</sup> National Chemistry Conference, Karachi, Pakistan, Dec. 4-6, 1998.
- Participated in the 7<sup>th</sup> International Symposium on Natural Product Chemistry, Karachi, Pakistan, from Dec. 28, 1997 to Jan. 1, 1998.

#### **Students Enrolled in M. Phil/PhD:**

Currently following students are enrolled in M. Phil / Ph. D. under my supervision.

<b>Name</b>	<b>Title</b>
<b>M. Riaz-uddin</b>	Computational Studies of Cholinesterase Inhibitors and Biological Studies of Related Enzyme.
<b>Abdul Wadood</b>	Computer-Aided Development of New Urease Inhibitors.
<b>Uzma Mahmood</b>	Structural and Molecular Modeling Studies on Cholinesterase Inhibitors
<b>Sobia Ahsan Halim</b>	Modeling Aided Lead Design of Cytokines Inhibitors
<b>Syed Tarique Moin</b>	Elucidating the Binding and Inhibition Mechanism of Lipoxigenase Inhibitors.
<b>Sadaf Iqbal</b>	Elucidating the Binding and Inhibition Mechanism of Different Metal Enzyme
<b>Waqas Uddin Khan</b>	Investigations on the Protein-Ligand Interactions Involved in T-cell Activation for Applications in Immune Therapies

**Master Thesis Supervised:**

<b>2008</b>		
Amal Jalil	Virtual Screening of Novel Non-Nucleoside HIV-1 Reverse Transcriptase	Department of Chemistry, University of Karachi
<b>2007</b>		
Saqib Faisal	Study of Protein-Ligand Interaction by Computational Chemistry Tools.	Department of Chemistry, University of Karachi
Bushra Jahangir	Structure Based 3D-QSAR Studies on Physostigmine Derivatives as Cholinesterase Inhibitors	Department of Chemistry, Urdu University
<b>2006</b>		
Lina Asif	3D-QSAR and Molecular Docking Studies of Podophyllotoxin Analogues as Tubulin Inhibitor	Department of Biochemistry, Jinnah University
Mehwish Aleem	Understanding The Antitumor Activity of Acylsulphonamide Derivatives Using Molecular Docking and 3D-QSAR Studies	Department of Biochemistry, Jinnah University
<b>2005</b>		
Erum Gul	Molecular Docking Studies of Urease Inhibitors	Department of Chemistry, University of Karachi
Sobia Halim	Different Docking Approach To Explore Protein-Ligand Interactions	Department of Biochemistry, Jinnah University
Mehrin Khan	Theoretical Analysis of The Active Site of Cholinesterase Enzyme.	Department of Biochemistry, Jinnah University

### **Research Support (as PI):**

- **INSPIRE** for the Talented Researcher Exchange Programme, British Council. (2009).
- **Collaboration** with the Theoretical Chemistry Department, University of Innsbruck, Austria in the Field of Computational Chemistry Research, Higher Education Commission, Pakistan, (2008).
- **Strengthening and Up gradation** of Computer-Aided Drug Design Laboratory at the Dr. Panjwani Center for Molecular Medicine and Drug Research, Higher Education Commission, Pakistan, (2007).
- *An In Silico* Approach to Discovering Novel Inhibitors for Helicobacter Pylori Urease: A Valid Target for Anti-Ulcer Therapy, **Higher Education Commission**, Pakistan, (2005)
- **Research Grants** to Active Scientists/ Technologists of Pakistan, Pakistan Science Foundation, (2005)
- **Collaboration** with the Pharmaceutical Biosciences, Pharmacology Department, Uppsala University in the Field of Proteo-Chemometrics Research, Higher Education Commission, Pakistan, (2005)
- **Start-up Funds** from Dr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical Sciences; University of Karachi (2004)