

Dr. M. Qaiser Fatmi



Professor & Team Leader

Computational Biology & Bioinformatics Group (CBBG), Department of Biosciences
COMSATS University Islamabad, Pakistan
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MY GOAL

I am a molecular modelist/computational chemist with over 16 years of post-PhD experience in research, 12 years in teaching and over 11 years in administration. I believe that *in silico* studies together with wet-lab experiments can lead to a better solution in healthcare, pharmaceutical and biotechnology sectors. I, therefore, focus on research where I can integrate these dry-lab studies with wet-lab experiments with an ultimate goal to serve the community in a better way. Moreover, I aim to integrate Artificial Intelligence in the field of organic chemistry, particularly in retrosynthesis analysis.

EDUCATION

Dr. Rer. Nat. (PhD) in March 2007 from the University of Innsbruck, Austria (Computational Chemistry)
M. Phil. Course in 2002 from the University of Karachi, Pakistan (Advanced Organic Chemistry)
M. Sc. in 2001 from the University of Karachi, Pakistan (Organic Chemistry)
B. Sc. in 1998 from the University of Karachi, Pakistan (Chemistry, Biochemistry, Molecular Biology)

EXPERIENCE

Head, Department of Biosciences, CUI, Islamabad, Pakistan, Nov. 2021 to Present
Professor, COMSATS University Islamabad, Islamabad, Pakistan, April. 2022 to Present
Associate Professor, COMSATS University Islamabad, Islamabad, Pakistan, March 2015 to April. 2022
Team Leader, Bioinformatics Group, CIIT, Islamabad, Pakistan, Jan. 2013 to Present
In-charge, Department of Biosciences, CIIT, Islamabad, Pakistan, Jan. 2013 to Sep. 2013
Assistant Professor, CIIT, Islamabad, Pakistan, Jul. 2011 to March 2015
Visiting Foreign Faculty, QAU, Islamabad, Pakistan, Feb. 2011 to Jul. 2011
Post-doctoral Employee, UCR, Riverside, USA, Jun. 2008 to Oct. 2010
Research Officer, ICCBS, Karachi, Pakistan, Mar. 2007 to May 2008

RESEARCH INTEREST & SKILLS

I am trained in different academic and commercial computational chemistry/structural bioinformatics tools based on windows and Linux OS. My study focuses on:

- Protein structure dynamics and function using biomolecular modelling and various MD simulations techniques
- Structure and ligand-based drug/inhibitor discovery using techniques involved in molecular docking and virtual screening etc
- Application of Artificial Intelligence/Machine Learning in Retro-Organic Synthesis

I have taught courses related to bioinformatics, protein chemistry, computational chemistry, computational protein design, general chemistry and organic chemistry.

ACHIEVEMENTS & HIGHLIGHTS

Following are my few achievements & highlights:

- ✚ **Successfully completed HEC NRPU** project as PI (around 2.1 million PKR).
- ✚ 1 patent submitted to Intellectual Property Organization of Pakistan
- ✚ Awarded Erasmus + International Credit Mobility fund to deliver a lecture series at Meddle East Technical University, Ankara, Turkey, 2017.
- ✚ Actively involved in teaching, research, administration & community services.
- ✚ **Published 50 papers** and **3 book chapters** with over 150 cumulative impact factors.
- ✚ **Supervised 40 BS and 32 MS** research students.
- ✚ **2 PhD students completed** thesis
- ✚ Currently supervising 3 MS and 2 PhD students.
- ✚ Active reviewer for PLoS One, Bioinformatics, EJMECH & JCSP etc.
- ✚ Honorarium for the good academic and administrative performance during year 2013, 2015, 2017 by COMSATS University.
- ✚ Research Productivity Award 2013, 2014, 2015, 2016, 2017, 2018 by COMSATS University.
- ✚ Letter of Appreciation for organizing a '2 Day Vice Chancellors forum' (11th to 12th June 2012).
- ✚ Awarded fund to attend a course on Agrochemicals and Drug Design, São Paulo, Brazil, (1st to 6th April 2012).
- ✚ HEJ start-up grant (2007-2008).
- ✚ OAD scholarships for Doctoral Program (2004-2007).
- ✚ Awarded HEC indigenous scholarship 2004 (declined).
- ✚ HEJ Fellowship (2001-2003).
- ✚ First Prize in poster presentation - 2nd Intl. and 12th National Chemistry Conference, University of Sindh, Jamshoro, Pakistan (4th to 6th Feb. 2002).
- ✚ Third Prize in model presentation - Science Exhibition of Fed. Government Urdu Science College (1998).

RESEARCH EXPERIENCES

Highlights:

- ✚ Over 16 years of post-PhD research experiences in Bioinformatics and Computational Chemistry.
- ✚ Over 3 years of research experiences in Organic Chemistry (Natural Product Chemistry, Biotransformation).
- ✚ Research Team Leader for Computational Biology and Bioinformatics Group (CBBG).
- ✚ Research Productivity Award 2013, 2014, 2015, 2016, 2017, 2018 by COMSATS Institute of Information Technology.
- ✚ Published 50 papers in ISI-indexed impact factor journals.

Dissertation Titles:

- ✚ **Ph.D.** Molecular Dynamics Simulations of Industrially and Biologically Relevant Ions.
- ✚ **M.Sc.** Microbial Transformation of Steroids and Antibiotic.

Team Leader "Computational Biology and Bioinformatics Group (CBBG)":

- ✚ Leading the Research Group and Establishing Research labs.
- ✚ Introduced PhD Bioinformatics Program
- ✚ Bioinformatics Accreditation from National Computing Education Accreditation Council (NCEAC), Higher Education Commission (HEC) Pakistan

Research Collaborations (Present & Past):

National:

- ✚ HEJ Research Institute of Chemistry, International Centre for Chemical and Biological Sciences (ICCBS), University of Karachi, Karachi
- ✚ Centre of Excellence for Molecular Biology (CEMB), The University of Punjab, Lahore
- ✚ Department of Chemistry, GC University, Lahore
- ✚ Department of Chemistry, Quaid-e-Azam University, Islamabad
- ✚ Department of Plant Breeding & Genetics - PMAS-Arid Agriculture University, Rawalpindi
- ✚ Department of Chemistry, University of Faisalabad, Faisalabad
- ✚ COMSATS Institute of Information Technology, Abbottabad Campus

International:

- ✚ Harvard Medical University, USA.
- ✚ MIT, USA.
- ✚ Faculty of Pharmacy, Universiti Teknologi MARA (UiTM), Malaysia.
- ✚ Atta-ur-Rahman Institute for Natural Products Discovery (AuRIns), Universiti Teknologi MARA (UiTM), Malaysia.
- ✚ Department of Biophysics, School of Medicine, Bahcesehir University, Istanbul, Turkey
- ✚ Department of Chemical and Biological Engineering, Koc University, Istanbul Turkey
- ✚ King Fahd Medical Research Center, King Abdulaziz University, Saudia Arabia.

Research Funding:

#	Title of the Project	Investigator	Funding Agency	Amount in Million PKR	Status
1.	Battle Against Cancer: <i>In Silico</i> Discovery of Potential Tyrosine Kinase Inhibitors	PI	HEC	2.1	Completed
2.	Structural Studies of Nitric Oxide Signaling: A Computational Approach for Discovering Cure of Cardiovascular Disorders	Co-PI	HEC	2.1	Approved & Running
3.	Strengthening Biotechnology Industry in the Country: Developing an educational tool kit for training undergraduate students as well as for research purposes: Lab to Commercialization	Co-PI	HEC	8.53	Approved & Running
4.	Identifying tryptophan synthase inhibitors to combat food borne disease (Salmonellosis): An in silico approach.	PI	TWAS-CIIT	0.5	Completed
5.	Regulating water transportation in Aquaporin: A step towards next-generation water filtration technology	PI	PSF	2.16	Submitted
6.	Ligand-Induced G-Quadruplex (G4) DNA Stabilization: A New Strategy for Cancer Therapy	PI	HEC	16.9	Declined
7.	A Multi-Target Drug Discovery Approach to Treat COVID-19	PI	PSF	8.28	Declined
8.	Targeting SARS-CoV-2 Main Protease as Treatment Strategy for COVID-19	PI	HEC	8	Declined
9.	Thermostability and Thermoactivity of Tryptophan Synthase: An In Silico Study	PI	PSF	2.02	Initially accepted, later declined upon request of budget reconsideration

Supervision of Research Students:

Summary:

Postdoc: 01 completed
 PhD: 02 completed, 02 enrolled
 MS: 32 completed, 02 enrolled
 BS: 40 completed, 04 enrolled

#	Student's Name	Dissertation Title	Status
PhD Students (4)			
1.	Shahr Bano Mirza (FA13-PBS-002)	Identification of Chemical- and Peptide-Based Inhibitors against Various Enzymes using State-of-the-Art Drug Discovery and Designing Technique	Completed (SP20)
2.	Andleeb Zahra (FA13-PBS-006)	Investigating the Role of Salivary miRNA as Potential Diagnostic Biomarker for Oral Cancers	Completed (FA21)
3.	Bushra Arif (SP18-PBS-001)	Discovery of Potential Inhibitor against Gut Microbial Protein involved in Colorectal Cancer	In Progress 10 th Semester

4.	Eisha Khilji (FA20-PBS-001)	Regulating Water Permeation in Aquaporin Z: Structure, Dynamics, Stability and Energetics Studies	In Progress 5 th Semester
MS Students (32)			
5.	Maryum Bibi (SP21-RBI-006)	Effects of Ionic Concentration on the Binding of G-Quadruplex with Stabilizing Small Molecules	FA22 (Completed)
6.	Shamsa Alam (SP20-RBI-017)	Water Permeation Effect Induced by Mutations at Isoleucine-164 in Aquaporin-2 (AQP-2) Using MD Simulations	SP22 (Completed)
7.	Zubair Hayat (SP20-RBI-009)	Molecular Dynamics Simulation Studies of Kras G-Quadruplexes DNA Inhibitors	FA21 (Completed)
8.	Safia Bibi (SP20-RBI-014)	Water Permeation Effect of Alanine65 Mutation Near NPA Motif of Aquaporin2	FA21 (Completed)
9.	Sabahat Zameer (SP20-RBI-013)	Exploring Water Permeation Effect in AQP2 due to Histidine172 Mutation in Ar/R Region	FA21 (Completed)
10.	Irum Shahzadi (FA19-RBI-009)	Water Permeation Effect Induced by Valine-168 Mutations Near the Constriction Region of Aquaporin 2	SP21 (Completed)
11.	Nasir Iqbal (SP19-RBI-012)	An Improved Approach for Retrosynthetic Analysis of Bioorganic Molecules by Deep Learning	FA20 (Completed)
12.	Aqsa Noureen (SP19-RBI-005)	Identification of Potential Ligands to Stabilize G-Quadruplexes located at Oncogenic K-RAS Gene	FA20 (Completed)
13.	Iqra (FA18-RBI-012)	Probing Water Permeation Effects of Tyrosine and Lysine Substituted Aromatic/Arginine Selectivity Filter of Aquaporin2	SP20 (Completed)
14.	Bareera Mehmood (FA18-RBI-008)	Water Channeling Effects due to Tryptophan and Lysine Mutations in Aromatic/Arginine Selectivity Filter of Aquaporin2	SP20 (Completed)
15.	Hafsa Anwar (FA18-RBI-008)	Exploring Water Permeation Effect due to Glutamine Mutation in NPA Motifs of Aquaporin2	SP20 (Completed)
16.	Maha Yousaf (FA18-RBM-002)	Discovering Potential Ligands to Stabilize Oncogenic G-Quadruplexes	SP20 (Completed)
17.	Fayez Shahzad (SP18-RBI-003)	Understanding Structure and Dynamics of Self-Assembling Short Peptides	FA19 (Completed)
18.	Maria Azhar (SP18-RBI-010)	Bacteriocins in Food Preservation: Peptide Identification and Binding Studies against various Enzymes	FA19 (Completed)
19.	Almas Gul Sikandari (SP18-RBI-008)	Identification of Potential Xylanase Inhibitors to Prevent Cell Wall Degradation in Plants	FA19 (Completed)
20.	Rabia Tesleem (FA17-RBM-019)	Anti-inflammatory Effects of Natural Compounds in Neuroinflammation	FA19 (Completed)
21.	Saher Tariq (FA17-RBI-003)	Designing and Development of Retrosynthetic Pathway Detection Tool for Bio-organic Molecules	SP19 (Completed)
22.	Aneela Yousaf (SP17-RBM-011)	In Silico and In Vivo Investigation of Potent Novel Polypharmacological Terpenoids for Alcohol Addiction	FA18 (Completed)
23.	Yusra Irshad (SP15-RBI-007)	The Effect of E2F4-DP2 Protein Phosphorylation on DNA Binding: A Molecular Dynamics Study	FA17 (Completed)
24.	Hira Jahangeer (SP15-RBI-007)	Effect of Gold Nanoparticle on Peptides Binding with DNA-domain of P53	FA17 (Completed)

25.	Mahrukh Imtiaz (SP15-RBI-007)	Glycan Chain- Induced Effect in Hydrogen Bonding Pattern of P-glycoprotein	FA16 (Completed)
26.	Maria Khalid (FA14-RBI-003)	Phosphorylation-Induced Conformational Changes in PAK/SH3 Protein Complex	SP16 (Completed)
27.	Wajid Khan (FA14-RBI-002)	Investigating Structure and Dynamics of Human Prion Protein Using Molecular Dynamics Simulation Approaches	SP16 (Completed)
28.	Ayesha Kanwal (SP14-RBI-004)	Extension of GraphMD: A User-Friendly Python-Based Interface for the Analysis of Molecular Dynamics Simulations' Results	FA16 (Completed)
29.	Tamseela Perveen (SP14-RBI-002)	Understanding the Structural and Dynamical Stability of Psychrophilic Tryptophan Synthase	FA15 (Completed)
30.	Aasia Saleem Khan (FA13-RBI-001)	Re-optimization, Pharmacokinetics and Spectral Prediction of Natural Products for Chemical Database of Pakistan	FA15 (Completed)
31.	Amina Khan (FA13-RBI-005)	Bioinformatics Analysis of the miRNA Target Genes in Gene Expression Profile of Chronic Kidney Diseases	FA15 (Completed)
32.	Ammarah Anwar (FA13-RBI-004)	A Comprehensive Analysis of Human Proteins' Binding Sites and its Implications for Drug Design	SP15 (Completed)
33.	Sadaf Shaheen (FA13-RBI-003)	Computational Analysis of Protein Binding Sites of Some Pathogenic Bacteria	SP15 (Completed)
34.	Maryam Latif (FA11-RBI-001)	Probing Ligand Interactions with different α -Glucosidase Orthologs	SP13 (Completed)
35.	Rashid Hussain (FA11-RBI-002)	Rationalizing Ligand-Protein Interactions for Cholinesterase Inhibitors Using Computational Methods	SP13 (Completed)
36.	Ayesha Babar (FA11-RBI-003)	<i>In Silico</i> Identification of Src Tyrosine Kinase Inhibitors	SP13 (Completed)
BS Students (40)			
37.	Fizza Rani (SP18-BSI-032) Habiba Mumtaz (SP18-BSI-033)	Potential of mean force of water permeating through AQP2 with mutated Valine-168	FA21 (Completed)
38.	Fakiha Balouch (SP18-BSI-006) Rabeea Afzal (SP18-BSI-017)	PMF Profile for Water permeation through AQP2 in Wild-Type and V168 with Hydrophobic Residue Substitution	FA21 (Completed)
39.	Zoya Iqbal (FA17-BSI-023) Suha Mishal (FA17-BSI-019)	MD simulation of E2F4-DP2 in complex with DNA	SP21 (In Progress)
40.	Ezna Ali (SP17-BSI-024) Mahnoor Imran (SP17-BSI-026)	Exploring Water Permeation Effect due to Histidine Mutation in ar/R region of Aquaporin 2	FA20 (Completed)
41.	Aamir Jan Khan (SP17-BSI-017) Muhammad Saqib Nadeem (FA16-BSI-008)	MDFast: A Python GUI Software for Analysis of MD Simulation Results	FA20 (Completed)

42.	Dua Fatima (FA16-BSI-002) Javaria Amin (FA16-BSI-027)	Temperature Effects on the Structure and Dynamics of G-Quadruplex DNA	SP20 (Completed)
43.	Ayesha Saeed Butt (SP16-BSB-013) Faiza Fatima (SP16-BSB-004)	Comparative Structure, Dynamics and Binding of Potential Inhibitor against various Mutated ABL Tyrosine Kinase Enzymes involved in CML	FA19 (Completed)
44.	Javeria Nazir (SP16-BSB-018) Fatima Zehra Hasan (SP16-BSB-033)	Ligand stabilization of c-kit G-Quadruplex DNA: An approach to treat gastrointestinal cancers	FA19 (Completed)
45.	Sonana Riaz (SP15-BSB-048) Salma Aslam (SP15-BSB-046)	Finding Potential Inhibitors for Prion Protein	FA18 (Completed)
46.	Ayesha (FA14-BSB-014) Nabeela Anwar (FA14-BSB-009)	Structure, Dynamics and Binding of Anticancerous Peptides with DNA-Binding Domain of P53 in the Presence of Gold Nanoparticle	SP18 (Completed)
47.	Amina Haq (SP14-BSB-030) Almas Gul Sikandari (SP14-BSB-018)	Battle against Cancer: Molecular Docking and Molecular Dynamics Simulation Studies for Drug Resistant T315I Mutant ABL Kinase Domain	FA17 (Completed)
48.	Aqsa Qureshi (SP14-BSB-044)	Identification of Tyrosine Kinase Inhibitors as Drug Candidates for Chronic Myeloid Leukemia: An <i>In Silico</i> Study	FA17 (Completed)
49.	Fayez Shahzad (FA13-BSB-009)	Finding New Indications of FDA Approved Drugs against Dengue Viral Proteins: A Structure-Based Approach	SP17 (Completed)
50.	Beenish (FA13-BSB-015) Rahma (FA13-BSB-020)	Repurposing Existing Drugs for New Indications against Dengue Viral Proteins: A Ligand-Based Approach	SP17 (Completed)
51.	Amir Khan (FA12-BSB-017)	Design and Development of National Cancer Registry of Pakistan	FA16 (Completed)
52.	Ujala Saeed (FA12-BSB-007) Aniza Aziz (FA12-BSB-002)	Peptide-Protein Binding and Induced Conformational Changes in Dengue NS3 Protein	FA16 (Completed)
53.	Hira Jahangir (SP12-BSB-010) Yusra Irshad (SP12-BSB-029)	Phosphorylation-Induced Conformational Changes in E2F4-DP2 Protein Complex: A Molecular Dynamics Study	FA15 (Completed)
54.	Khushboo Akhlaq (SP11-BSB-014)	Improving the Binding Affinity of β -Secretase 1 Inhibitors through Virtual Derivatization using Flexible Docking Approach	FA14 (Completed)
55.	Sumaira Malik (SP11-BSB-031) Itrat Rubab (SP11-BSB-012)	<i>In Silico</i> Characterization and Analysis of miRNA Involved in Oral Cancer	FA14 (Completed)

56.	Mahrukh Imtiaz (SP11-BSB-016)	Computational Designing of Peptide Inhibitors Against NS3 Protein of Dengue Virus	FA14 (Completed)
57.	Kamilia Tasleem (SP11-BSB-013)	Virtual Screening of NS5 Protein of Dengue Virus: A Ligand-Based Pharmacophore Modeling Approach	FA14 (Completed)
58.	Hira Batool (SP10-BSB-013)	GraphMD: A python Based Interface for the Graphical Analysis of Molecular Dynamics Simulations' Results of Proteins and their Complexes	FA13 (Completed)
59.	Abeerah Nawaz (SP08-BSB-002)	The Effect of Different DNA Gyrase Conformations on Ligand Binding	FA12 (Completed)
60.	Adil Bhatti (FA08-BSB-004)	Identification of Spleen Tyrosine Kinase Inhibitors using Structure-Based Drug Design Approaches and Preliminary Studies of Mutational Dynamics	SP12 (Completed)
61.	Ammarah Anwar (FA08-BSB-046) Sana Vaqar (FA08-BSB-030)	Structural and Dynamical Comparison of Hyperthermophilic and Mesophilic Tryptophan Synthase: Probing through Molecular Dynamics Simulations and Molecular Docking Studies	SP12 (Completed)

Supervision of Postdoctoral Fellows:

#	Fellow's Name	Research Topic	Funding	Country
01	Dr. Mohammed Suleiman Zaroog	Identifying tryptophan synthase inhibitors to combat food borne disease (Salmonellosis): An <i>in silico</i> approach.	TWAS-CIIT	Sudan

Co-Supervision of Research Students:

#	Student's Name	Dissertation Title	Status
PhD Students (1)			
01	Rashid Hussain (Forman Christian College University, Lahore)		SP23 (Completed)
MS Students (3)			
01	Arifa Bibi (Sardar Bahadur Khan Women University, Quetta)	Structure and Dynamics of Mutated Tyrosine Kinase (T315I) in Complex with Potential Inhibitors	SP21 (Completed)
02	Humaira Bibi (Sardar Bahadur Khan Women University, Quetta)	Identification of Withanolides and Related Compound as Potential Inhibitor of Dengue Protein: A Combined Molecular Docking and Molecular Dynamics Simulation Study.	SP20 (In Progress)

03	Shahr Bano Mirza (FA11-RBI-004)	3D Structure Optimization and Database Development for Pakistani Relevant Natural Products and their Derivatives	SP13 (Completed)
BS Students (>19)			
Over 19 students have been co-supervised			

Research Posters:

- ✚ "The role of oligomerization and synergistic regulations in tryptophan synthase's function."
M. Qaiser Fatmi and Chia-en A. Chang.
São Paulo School of Advanced Science (ESPCA), Campinas, São Paulo, Brazil
(April 1-6, 2012).
- ✚ "Discovering Drug Candidates for the alpha-subunit of Tryptophan Synthase: From Docking, Molecular Dynamics Simulations, to Experiments."
M. Qaiser Fatmi, Wai M. Thant, Sunny Lee, Demetri Niks, Michael F. Dunn, Chia-en A. Chang.
239th ACS National Meeting & Exposition, San Francisco, California, USA
(March 21-25, 2010).
- ✚ "Application of the new quantum mechanical charge field (QMCF) molecular dynamics formalism to structure and dynamics of TiO₂⁺ complex."
M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode.
42nd Symposium on Theoretical Chemistry, Humboldt University, Erkner, Germany
(Sep. 3-6, 2006).
- ✚ "QM/MM MD Simulation Study of the Pentaquozinc(II)-amine Complex in Aqueous Solution"
M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode.
10th International Symposium on Natural Product Chemistry (ISNPC-10), Karachi, Pakistan
(Jan. 6-9, 2006).
- ✚ "An extended ab initio QM/MM MD simulation of Zn(II) in aqueous solution and temperature effects on the structure and dynamics of [Zn(H₂O)₆]²⁺ complex."
M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode.
2nd Annual CMBI Meeting (Center for Molecular Biosciences Innsbruck), Vill, Austria
(Sep. 30- Oct. 7, 2005).
- ✚ "An extended ab initio QM/MM MD simulation of Zn(II) in aqueous solution and temperature effects on the structure and dynamics of [Zn(H₂O)₆]²⁺ complex."
M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode.
41st Symposium on Theoretical Chemistry, University of Innsbruck, Innsbruck, Austria
(Sep. 5-7, 2005).
- ✚ "Microbial Transformation of Deoxycholic Acid."
M. Qaiser Fatmi, M. Iqbal Choudhary, Farzana Shaheen, Atta-ur-Rahman.
H.E.J.-COMSTECH (CPC)-TWAS International Workshop on the development of medicines from plants,
University of Karachi, Karachi, Pakistan
(Sep. 8-13, 2003).
- ✚ "Stereo- and Regio-selective Microbial Transformation of Norgestrel."
M. Qaiser Fatmi, M. Iqbal Choudhary, Atta-ur-Rahman, Farzana Shaheen.
3rd International and 13th National Chemistry Conference, University of Karachi, Pakistan (Dec. 28-31, 2002).
- ✚ "Fungal Transformation of 4-Androstene-3,17-dione."

M. Qaiser Fatmi, M. Iqbal Choudhary, Sadia Sultan, Rahat Azhar Ali, Atta-ur-Rahman, Farzana Shaheen.
7th Eurasia Conference on Chemical Sciences, Karachi, Pakistan
(March 9-12, 2002).



"Microbial Oxidation of 4-Androstene-3,17-dione."

M. Qaiser Fatmi, M. Iqbal Choudhary, Sadia Sultan, Rahat Azhar Ali, Atta-ur-Rahman, Farzana Shaheen.
2nd International and 12th National Chemistry Conference, University of Sindh, Jamshoro, Pakistan
(Feb. 4-6, 2002).



"Glycolysis and TCA Cycle."

M. Qaiser Fatmi.

Science Exhibition of Federal Government Urdu Science College, Karachi, Pakistan (1998).

TEACHING EXPERIENCES

Highlights:

- ✚ Over 13 years of teaching experiences in Chemistry, Bioinformatics and Computational Chemistry at university level students.
- ✚ Student teaching evaluation is "Excellent".
- ✚ Designed "Biomolecular Modeling" and "Computational Protein Design" courses for MS/PhD students.
- ✚ Introduced PhD Bioinformatics Program at the Department of Biosciences, CUI.

Course Details:

Course Title	Level	Credit Hours	Semesters	University
Retrosynthesis	MSc	3(3,0)	SP11	QAU
Computational Chemistry	MPhil/PhD	3(3,0)	SP11	QAU
Protein Chemistry	MS/PhD	4(4,0)	FA11, FA12	CUI
Bioinformatics	MS/PhD	3(3,0)	FA11	CUI
Special Topics in Bioinformatics	MS/PhD	3(3,0)	FA11, FA13, FA14	CUI
Bioinformatics Colloquium	BS	1(1,0)	FA11, SP12, SP20	CUI
General Chemistry with lab	BS	4(3,1)	SP12, FA13, SP22, FA22	CUI
Biomolecular Modeling	MS/PhD	3(3,0)	SP13, SP15, SP16, SP17, SP18, FA18, FA19, SP20, FA20, SP21, FA21, SP23	CUI
Computational Protein Design	MS/PhD	3(3,0)	FA15, FA16, FA17, SP19, SP20	CUI

QAU = Quaid-i-Azam University Islamabad; CUI = COMSATS University Islamabad

ADMINISTRATIVE EXPERIENCES

Highlights:

- ✚ Over 15 years of university/departmental/group administration experiences.
- ✚ Awarded honorarium for the excellent performance in 2013 and 2015 by the university.
- ✚ Awarded appreciation letter for actively organizing Vice Chancellor meeting during 2012.

Job Details:

#	Title for Administrative Posts	Period	Main Job Description
1.	Head, Department of Biosciences	FA21 – Present	<ul style="list-style-type: none"> – Running the Department – Report to In-charge Campus/Rector
2.	Counsellor BS students	FA11 – FA15 FA18 – FA20	<ul style="list-style-type: none"> – Counselling students – Meet students periodically – Resolve students' issues – Motivate students for academia, sports, career etc – Report to Head of Department
3.	Member & Deputy Convener Convocation Arrangement Team	SP18	<ul style="list-style-type: none"> – Convocation Organization – Coordination between members – Report to Convener
4.	Member Departmental Board of Studies (BoS), CIIT	FA15 - Present	<ul style="list-style-type: none"> – Discussion on Departmental Academic matters & policy proposal – Report to Chairperson
5.	Secretary Departmental Tenure Track Review Committee (DTRC), CIIT	SP16 - FA18 SP19 – FA21	<ul style="list-style-type: none"> – Document the minutes – Coordination between DTRC members – Report to Convener
6.	Member Self-Assessment Report (SAR), Bioinformatics Program, CIIT	SP16 – FA17 FA19 – FA21	<ul style="list-style-type: none"> – Preparing SAR for Bioinformatics Program – Report to Head of Department
7.	Member Departmental Advisory Committee (DAC), Biosciences, CIIT	FA13 – Present	<ul style="list-style-type: none"> – Initial Evaluation of MS/PhD Synopses – Recommendations regarding academic improvement – Report to Convener
8.	Member Campus Tenure Track Committee	FA18 – SP20	<ul style="list-style-type: none"> – Recommendations to resolve TTS matters – Report to Convener
9.	Young Advisor to Rector CIIT	FA14 – FA17	<ul style="list-style-type: none"> – Discussion on CIIT/CUI vision – Innovative ideas to improve the quality education at campus. – Ideas to improve the teaching, research and services at CIIT/CUI. – Report to Rector
10.	Member Departmental Academic Regulatory Committee (DARC), CIIT	FA13 – FA17	<ul style="list-style-type: none"> – Overview course distribution to Faculty – Monitor the quality of teaching and lab. – Evaluate exam paper and marks distribution
	Focal Person Departmental Academic	SP18 – SP21	<ul style="list-style-type: none"> – Monitor students' attendance – Monitor online portal

	Regulatory Committee (DARC), CIIT		<ul style="list-style-type: none"> – Address any teaching problem reported by students or by faculty members – Report to Convener
11.	In-charge Admission Campaign Biosciences Department, CIIT	FA13 – FA15	<ul style="list-style-type: none"> – Run admission campaign – Meet students in colleges and schools – Invite students for demonstration – Report to Head of Department
12.	Member Examination Panel Undergraduate/Graduate Bioinformatics, CIIT	FA13 – FA21	<ul style="list-style-type: none"> – Assess the quality of research and presentation of BS/MS thesis – Grading research of students – Report to Head of Department
13.	Convener Interview Panel for MS Bioinformatics Admission, CIIT	FA13 – FA21	<ul style="list-style-type: none"> – Evaluate the eligibility and ability of students – Based on merit, recommend student for admission – Report to Head of Department
14.	Team Leader Bioinformatics Division, CIIT	SP13 - Present	<ul style="list-style-type: none"> – Lead the Computational Biology & Bioinformatics Group (CBBG) – Review and improve curricula – Introduce new courses and degree programs – Meeting bioinformatics faculty members periodically – Resolve students' issues related to research, career etc
15.	In-charge (Head) Department of Biosciences, CIIT	Jan 2013 - Sep 2013	<ul style="list-style-type: none"> – Run the Biosciences Department – Report to Director CIIT/CUI
16.	Member Review Committee for Exam disputed paper other than cheating, CIIT	SP13 - FA13	<ul style="list-style-type: none"> – Resolve the issue related to disputed exam papers – Report to the Convener
17.	In-charge Undergraduate Program of Biosciences, CIIT	FA11 - FA12	<ul style="list-style-type: none"> – Course distribution to faculty – Prepare semester schedule and timetable – Prepare examination date sheet – Resolve students' issues related to academia, teaching and research – Report to Head of Department
18.	In-charge Departmental Transport Committee, CIIT	FA11 - FA11	<ul style="list-style-type: none"> – Arrange transport for students and faculty for official purpose – Arrange transport for study tour and fun trips
19.	Lab Administration, UCR, USA	Jun 2008 – October 2010	<ul style="list-style-type: none"> – Linux machine administration – Software installation and networking – Facilitate other lab researchers – Report to Advisor (PI)

CIIT = COMSATS Institute of Information Technology (Now COMSATS University Islamabad; CUI)

SERVICES

Journal Reviewer:

- ✦ Journal of Pakistan Chemical Society
- ✦ PLoS One
- ✦ Bioinformatics
- ✦ European Journal of Medicinal Chemistry
- ✦ Computational Biology and Chemistry
- ✦ Egyptian Journal of Medical Human Genetics
- ✦ Computers in Biology and Medicine

Project Reviewer:

- ✦ Higher Education Commission of Pakistan (HEC)
- ✦ Pakistan Science Foundation (PSF)
- ✦ Internal Projects of Virtual University (VU)
- ✦ Internal Projects of COMSATS University Islamabad (CUI)

Member:

- ✦ Jury Member for National Awards of Young Scientists (NAYS) since 2011-2013
- ✦ Member National Testing Services (NTS) for Bioinformatics, 2013
- ✦ Nominated Member for National Curriculum Revision Committee (NCRC) of Higher Education Commission Pakistan in 2014.

Workshop Organization:

- ✦ "Workshop on Molecular Modeling in Chemistry and Beyond"
Department of Chemistry, Quaid-i-Azam
University, Islamabad, Pakistan,
(May 27-29, 2011).
- ✦ "Workshop on *In Silico* Tools in Medicinal Chemistry"
Department of Chemistry, Quaid-i-Azam
University, Islamabad, Pakistan,
(Dec. 22-25, 2011).

Community Services:

- ✦ Participant of "Adapt a tree" drive by COMSATS University
- ✦ Awareness of secondary school's students for research & innovation
- ✦ Computational chemistry trainer at www.ScientificPakistan.com

CERTIFICATE COURSES ATTENDED

- ✚ Five days training on “Workshop for Academic Leaders” conducted by Faculty Development Academy (FDA), CUI, Islamabad.
(Dec 14, to 18, 2020)
- ✚ Three months courses for Freelancing and Wordpress (Web designing) offered online by the ministry of Science and Virtual University through www.digiskills.pk.
(February to May 2020)
- ✚ “Advanced Topics in Computational Biology – Agrochemicals and Drug Design”,
Conducted by Prof. Dr. Goran Neshich at Embrapa, São Paulo School of Advanced Science (ESPCA),
Campinas, São Paulo, Brazil
(1st to 6th April 2012).
- ✚ “Students' Counseling for Teachers” conducted by Faculty Development Academy, CIIT Islamabad.
(8th to 12th August 2011).
- ✚ “An Introduction to Bioinorganic and Medicinal Chemistry of Metals”,
Conducted by Dr. M. Maroof Tahir (USA) at the HEJ Research Institute of Chemistry
(17th to 31st May 2003).
- ✚ “Biochemical Basis of Diabetes and Ageing”,
Conducted by Dr. Nessar Ahmed (UK) at the HEJ Research Institute of Chemistry
(15th to 24th April 2003).
- ✚ “Animal Cell Culture”,
Conducted by Dr. Rafat Ali Siddiqui (USA) at the HEJ Research Institute of Chemistry
(23rd December 2002 to 3rd January 2003).
- ✚ “Lecture Series on Scientific Integrity”,
Conducted by Dr. Mohsin Raza (Pak.) at the HEJ Research Institute of Chemistry
(2nd to 16th September 2002).
- ✚ “Bangladesh-Pakistan Binational Seminar on Natural Product Chemistry”,
Organized by HEJ Research Institute of Chemistry
(24th to 26th September 2002).

ORAL TALKS

- ✚ “Molecular Dynamics Simulation: Application & Scope” (**Invited Speaker**)
M. Qaiser Fatmi
Conference on “Molecular Dynamics in Soft Matter and Biological Physics” at Lahore University of Management Sciences (LUMS). SBASSE Dean’s Smart Room, Lahore.

(February 13-14, 2020)

- ✚ “The Role of Molecular Dynamics Simulation in Computer-Aided Drug Discovery” (**Key Note Speaker**)
M. Qaiser Fatmi
GPGC Mandian Conference & Workshop 2020 on "Augmenting Research Writing Skills Tools and Technologies Transforming Life Sciences" at Govt Post Graduate College Mandian Abbottabad.
(January 9-11, 2020)
- ✚ “How Computational Chemistry can help in Drug Discovery: Brief Discussion on Two Running Projects” (**Invited Speaker**)
M. Qaiser Fatmi
1st International Conference on Medicinal Chemistry & Drug Discovery, COMSTECH secretariat, Islamabad, Pakistan.
(October 18-19, 2018)
- ✚ “Research Activities at Biosciences Department: A Focus on the Application of Molecular Dynamics Simulations” (**Nominated**)
M. Qaiser Fatmi
Second Joint Pakistan-Belarus Young Scientists Forum (YSF), COMSATS Institute of Information Technology, Islamabad, Pakistan
(December 20, 2017)
- ✚ “Computational Techniques in Drug Discovery: A Focus on MD Simulation Approach” (**Invited Speaker**)
M. Qaiser Fatmi
Symposium on Computer Aided Drug Design, Research Center for Modeling and Simulation (RCMS), National University of Sciences and Technology (NUST), Islamabad, Pakistan
(September 27, 2017)
- ✚ “A Talk Series on Structural Bioinformatics”
M. Qaiser Fatmi
Department of Biological Sciences, Middle East Technical University, Ankara, Turkey
(March 05-10, 2017)
- ✚ “Molecular Dynamics Simulations: An Introduction” (**Invited Speaker**)
M. Qaiser Fatmi
Two Days Workshop on “Bioinformatics and Computational Drug Designing”, Kinnaird College, Lahore, Pakistan
(January 27-28, 2017)
- ✚ “Inhibitors against dengue NS3 protein: *In silico* study of eighteen million molecules” (**Invited Speaker**)
M. Qaiser Fatmi
4th International Conference on Biological and Computer Sciences (C-BICS 2016), Capital University of Science & Technology, Islamabad, Pakistan
(December 17th, 2016)
- ✚ “Computational Environmental Chemistry: An Area Pakistan Needs Special Focus” (**Nominated**)
M. Qaiser Fatmi
4th International Conference on Environmental Horizon: Valuing and Conserving Nature, University of Karachi, Pakistan
(January 08-10, 2016)

- ✚ "Understanding Protein Function using Bioinformatics Tools: Tryptophan Synthase as a case study"
M. Qaiser Fatmi
Symposium on Epigenetics and Computational Biology, University of Gujrat, Pakistan
(May 15, 2015)

- ✚ "Understanding Protein Function through Ligand-Induced Conformational Changes, Oligomerization and Synergistic Regulation of Tryptophan Synthase "
M. Qaiser Fatmi, Chia-en A. Chang.
6th One day workshop on impact of bioinformatics in life sciences, MAJU, Islamabad, Pakistan
(May 09, 2015)

- ✚ "Protein 3D structure prediction"
M. Qaiser Fatmi
Department of Chemistry, Quaid-i-Azam, University, Islamabad, Pakistan
(Dec. 22-25, 2011).

- ✚ "Introduction to molecular mechanics and its applications"
M. Qaiser Fatmi
Department of Chemistry, Quaid-i-Azam, University, Islamabad, Pakistan
(May 27-29, 2011).

- ✚ "Homology modeling of alpha-glucosidase"
M. Qaiser Fatmi
Department of Chemistry, Quaid-i-Azam University, Islamabad, Pakistan
(May 27-29, 2011).

- ✚ "Driving forces behind allosteric and synergistic regulations in tryptophan synthase"
M. Qaiser Fatmi, Rizi Ai, Chia-en A. Chang.
239th ACS National Meeting & Exposition, San Francisco, California, USA
(March 21-25, 2010).

- ✚ "Synergistic regulation and ligand-induced conformational changes of tryptophan synthase."
M. Qaiser Fatmi, Chia-en A. Chang.
237th ACS National Meeting & Exposition, Salt Lake City, Utah, USA
(March 22-26, 2009).

SCIENTIFIC MEMBERSHIP

- ✚ American Chemical Society (Active member 2008 - 2011)

LIST OF PUBLICATIONS

Summary:

Total Published Papers (ISI-Indexed):	50
JCR Impact Factor (Clarivate Analysis):	>140
Submitted (ISI-Indexed)	2
In Preparation	3
h-Index:	18 (Google Scholar, as of April 2023)
i10-Index:	28 (Google Scholar, as of April 2023)
Total Citation:	992 (Google Scholar, as of April 2023)
ORCID:	0000-0001-5680-8103
Google Scholar Link:	https://scholar.google.com/citations?user=4F0SjE8AAAAJ&hl=en

#	Name of Authors	Complete Name of Journal and address with ISSN (Print) No.	Title of the Publication	Vol. No. & Page No.	Year Published
1.	Jumi Das, M. Qaiser Fatmi, Mary Devi, Namram Sushindrajit Singh, Akalesh Kumar Verma	Journal of Molecular Structure	Antitumor activity of cordycepin in murine malignant tumor cell line: An in vitro and <i>in silico</i> study	Under Review	
2.	Andleeb Zahra; Muhammad Jawad Khan; Ghulam Rabia; Syeda Aba Ali; Sana Mumtaz; Hassaan Mehboob Awan; Muhammad Qaiser Fatmi	Molecular Genetics and Genomics	Expression of salivary miRNA-300 and miRNA-340-5p in oral cancer patients of Pakistan	Under Review	
3.	Maria Azhar, Maha Yousaf, Saima Maher, M. Qaiser Fatmi*	Applied Biochemistry and Biotechnology	Discovering Potential Bacteriocins against <i>Pseudomonas fragi</i> : A Subtractive Proteomics and Molecular Dynamics Simulation Study for Food Preservation	1-18 http://doi.org/10.1007/s12010-023-04509-7	2023
4.	Maha Yousaf, Dua Fatima, Javaria Amin, Aqsa Noureen, M. Qaiser Fatmi*	Journal of Biomolecular Structure & Dynamics	Discovering Potential Stabilizers for KRAS22RT G-Quadruplex DNA: An Alternative Next Generation Approach to Treat Pancreatic Cancer	1-12 http://doi.org/10.1080/07391102.2023.2174188	2023
5.	Kamal A Qureshi, Faizul Azam, M. Qaiser Fatmi, Mahrukh Imtiaz, Dinesh K Prajapati, Pankaj Rai, Mariusz Jaremko, Emwas A-H, Gamal Elhassan	PeerJ	<i>In vitro</i> and <i>in silico</i> evaluations of actinomycin X ₂ and actinomycin D as potent anti-tuberculosis agents	11, e14502 http://doi.org/10.7717/peerj.14502	2023
6.	Ahsanullah Unar, Mahrukh Imtiaz, Truong Tan Trung, Maria Rafiq, Muhammad Qaiser Fatmi*, Tassadaq Hussain Jafar*	Current Bioinformatics	Structural and Functional Analyses of SARS COV-2 RNA-dependent RNA polymerase Protein and Complementary vs. Synthetic Drugs against COVID-19, and the Exploration of Binding Sites for Docking, Molecular Dynamics Simulation, and Density Functional	17, 632 - 656	2022

			Theory Studies		
7.	Kamal A Qureshi*, Mahrukh Imtiaz, Ibrahim Al Nasr, Waleed S. Koko, Tariq A. Khan, Mariusz Jaremko, Syed Mahmood, M. Qaiser Fatmi*	Antibiotics	Antiprotozoal Activity of Thymoquinone (2-Isopropyl-5-methyl-1,4-benzoquinone) for the Treatment of Leishmania major-Induced Leishmaniasis: In Silico and In Vitro Studies	11, 1206	2022
8.	Rashid Hussain, Hira Khalid, M. Qaiser Fatmi	Pure and Applied Chemistry	HCV genotype-specific drug discovery through structure-based virtual screening	PAC 2021-1104	2022
9.	Farmanullah, Nadia Khurshid, M. Qaiser Fatmi , Muhammad Saeed, Peter Loidl	PLOS One	Mutations in the acetylation hotspots of Rbl2 are associated with increased risk of breast cancer	PONE-D-22-02667R2, e0266196	2022
10.	Kamal A Qureshi, Mahrukh Imtiaz, Adil Parvez, Pankaj K Rai, Mariusz Jaremko, Abdul-Hamid Emwas, Avinash D Bholay, Muhammad Qaiser Fatmi*	Antibiotics	<i>In Vitro</i> and <i>In Silico</i> Approaches for the Evaluation of Antimicrobial Activity, Time-Kill Kinetics, and Anti-Biofilm Potential of Thymoquinone (2-Methyl-5-propan-2-ylcyclohexa-2, 5-diene-1, 4-dione) against Selected Human Pathogens	11, 79	2022
11.	M. M. Alam, A. Ikram, N. Mahmood, S. Sharif, S. Shaukat, M. Qaiser Fatmi , M. Angez, A. Khurshid, L. Rehman, R. Akhtar, G. Mujtaba, Y. Arshad, M. S. Rana, A. Yousaf, S. S. Z. Zaidi, M. Salman	The Journal of Infectious Diseases	Conserved Antigenic Structure of Contemporary Wild Poliovirus Type 1 Strains Endemic in Pakistan	226, 843–851	2022
12.	Rashid Hussain, Hira Khalid, and M. Qaiser Fatmi	Journal of Computational Biophysics and Chemistry (Formerly known as Journal of Theoretical and Computational Chemistry)	Molecular Modeling Approach of Serine Protease NS3-4A Genotype 3a as A Potential Drug Target of Hepatitis C Virus: Homology Modeling and Virtual Screening Study	20, 631-639	2021
13.	Salma Saeed Khan, Yi Shen, M. Qaiser Fatmi , Robert E. Campbell and Habib Bokhari	Biomolecules	Design and Prototyping of Genetically Encoded Arsenic Biosensors Based on Transcriptional Regulator AfArsR	11, 1276	2021
14.	Kamal A. Qureshi, Ibrahim Al Nasr, Waleed S. Koko, Tariq A. Khan, M. Qaiser Fatmi , Mahrukh Imtiaz, Riaz A. Khan, Hamdoon A. Mohammed, Mariusz Jaremko, Abdul-Hamid Emwas, Faizul Azam, Avinash D. Bholay, Gamal O. Elhassan, and Dinesh K. Prajapati	Antibiotics	In Vitro and In Silico Approaches for the Antileishmanial Activity Evaluations of Actinomycins Isolated from Novel Streptomyces smyrnaeus Strain UKAQ_23	10, 887	2021

15.	Sobia Ahsan Halim, Ajmal Khan, Abdul Wadood, Zaheer-ul-Haq, Sadaf Naeem, Almas Gul Sikandari, M. Qaiser Fatmi*	Biomolecules	Structure based virtual screening of Tumor Necrosis Factor- α Inhibitors by Chemoinformatics Approaches and Biomolecular Simulation	11, 329	2021
16.	Amina Khan, Andleeb Zahra, Sana Mumtaz, M. Qaiser Fatmi* , Muhammad Jawad Khan*	Current Bioinformatics	Integrated in silico analysis to study the role of microRNAs in detection of chronic kidney diseases	15, 144-154	2020
17.	Muhammad Taha, Sadia Sultan, Muhammad Herizal, M. Qaiser Fatmi , Manikandan Selvaraj, Kalavathy Ramasamy, Sobia Ahsan Halim, Siong Meng Lim, Fazal Rahim, Adeeb Shehzad	Journal of Saudi Chemical Society	Synthesis, anticancer, molecular docking and QSAR studies of benzoylhydrazone	23, 1168-1179	2019
18.	Amna Iqbal, Shahrukh Malik, Syed M Nurulain, Kamil Musilek, Kamil Kuca, Huba Kalasz, M. Qaiser Fatmi*	Chemico-Biological Interaction	Reactivation potency of two novel oximes (K456 and K733) against paraoxon-inhibited acetyl and butyrylcholinesterase: In silico and In vitro models	310, 108735	2019
19.	Tamsila Parveen, M. Kamran and M. Qaiser Fatmi*	Archives of Biochemistry and Biophysics, ISSN: 0003-9861	Structural and Dynamical Thermostability of Psychrophilic Enzyme at Various Temperatures: Molecular Dynamics Simulations of Tryptophan Synthase.	663, 297-305	2019
20.	A Nigar, M Shabbir, Z Akhter, S Sabahat, M. Qaiser Fatmi , M Bolte, I Ahmad, NK Janjua, S Mehmood	Journal of Molecular Structure, ISSN: 0022-2860	Synthesis, characterization, docking and electrochemical studies of nitroaromatic amide.	1176, 791-797	2019
21.	M Umair, BH Abbasi, S Sharif, MM Alam, MS Rana, G Mujtaba, Y Arshad, M. Qaiser Fatmi , SZ Zaidi	PLoS One, ISSN: 1932-6203 (Electronic)	High prevalence of G3 rotavirus in hospitalized children in Rawalpindi, Pakistan during 2014.	13, e0195947	2018
22.	A Zahra, I Rubab, S Malik, A Khan, MJ Khan, M. Qaiser Fatmi*	BioMed Research International, ISSN: 2314-6133	Meta-Analysis of miRNAs and Their Involvement as Biomarkers in Oral Cancers.	2018, Article ID 8439820	2018
23.	M Arshad, M. Qaiser Fatmi , K Musilek, A Hussain, K Kuca, G Petroianu, H Kalasz, SM Nurulain	Toxicology Mechanisms and Methods, ISSN: 1537-6516	In silico and in vitro evaluation of two novel oximes (K378 and K727) in comparison to K-27 and pralidoxime against paraoxon-ethyl intoxication.	28, 62-68	2018
24.	A Iqbal, HM Siddiqi, Z Akhter, M. Qaiser Fatmi	Journal of Molecular Structure, ISSN: 0022-2860	Design and characterization of novel bis-benzamide liquid crystalline materials.	1151, 135-141	2018
25.	Shaher Bano Mirza, Ramin Ekhteiari Salmas, M. Qaiser Fatmi , Serdar Durdagi	Journal of Enzyme Inhibition and Medicinal Chemistry, ISSN: 1475-6366	Discovery of Klotho peptide antagonists against Wnt3 and Wnt3a target proteins using combination of protein engineering, protein-protein docking, peptide docking and molecular dynamics simulation.	32, 84-98	2017
26.	Muhammad Zaheer, Zareen Akhter, Asghari Gul, Misbah Tauseef,	Journal of the Chemical Society of Pakistan,	Biological evaluation of newly synthesized Schiff Bases: Crystal	38 737-748	2016

	Bushra Mirza, Michael Bolte, M. Qaiser Fatmi	ISSN: 0253-5106	Structure complemented by DFT calculation.		
27.	Shaher Bano Mirza, Ramin Ekhteiari Salmas, M. Qaiser Fatmi* , Serdar Durdagi	Journal of Molecular Graphics and Modelling, ISSN: 1093-3263	Virtual Screening of Eighteen Million Compounds against Dengue Virus: Combined Molecular Docking and Molecular Dynamics Simulations Study.	66, 99-107	2016
28.	Farukh Jabeen, Syeda Aaliya Shehzadi, M. Qaiser Fatmi , Sobia Shaheen, Lubna Iqbal, Nighat Afza, Siva S. Panda, Farzana Latif Ansari	Bioorganic & Medicinal Chemistry Letters, ISSN: 0960-894X	Synthesis, in vitro and computational studies of 1,4-disubstituted 1,2,3-triazoles as potential α -glucosidase inhibitors.	26, 1029-1038	2016
29.	Shahar Bano Mirza, Habib Bokhari, M. Qaiser Fatmi*	Current Computer-Aided Drug Design, ISSN: 1573-4099	Exploring Natural Products from the Biodiversity of Pakistan for Computational Drug Discovery Studies: Collection, Optimization, Design and Development of A Chemical Database (ChemDP).	11, 102-109	2015
30.	Muhammad Taha, Nor Hadiani Ismail, Ajmal Khan, Syed Adnan Ali Shah, Ammarah Anwar, Sobia Ahsan Halimf, M. Qaiser Fatmi , Syahrul Imran, Fazal Rahim, Khalid Mohammed Khan	Bioorganic & Medicinal Chemistry Letters, ISSN: 0960-894X	Synthesis of novel derivatives of oxindole, their urease inhibition and molecular docking studies.	25, 3285-3289	2015
31.	Shilu Mathew, Kaneez Fatima, M. Qaiser Fatmi , Govindaraju Archunan, Muhammad Ilyas, Nargis Begum, Ishtiaq Qadri	PLoS One, ISSN: 1932-6203 (Electronic)	Computational docking study of p7 ion channel from HCV Genotype 3 and Genotype 4 and its interaction with natural compounds.	10, e0126510.	2015
32.	Muhammad Taha, Nor Hadiani Ismail, Salima Lalani, M. Qaiser Fatmi , Khalid Mohammed Khan, Salman Siddiqui, Momin Khan, Muhammad Iqbal Choudhary.	European Journal of Medicinal Chemistry, ISSN: 0223-5234	Synthesis of Novel Inhibitors of α -Glucosidase Based on Benzothiazole Skeleton Containing Benzoydrazone Moiety and their Molecular Docking Studies.	92, 387-400	2015
33.	Muhammad Sulaman Nawaz, Zahida Parveen, Liyong Wang, Sajid Rashid, M. Qaiser Fatmi , Mohammad A. Kamal	CNS & Neurological Disorders Drug Targets, ISSN: 1871-5273	Computational Study of Human Tyrosine Hydroxylase Mutants to Uphold [4-(Propan-2-yl) Phenyl]Carbamic Acid as a Potential Inhibitor.	13, 1169-1174	2014
34.	Khushi Muhammad, M. Qaiser Fatmi , Shahid Hameed	Molecular Crystals and Liquid Crystals, ISSN: 0026-8941	Theoretical Calculations on Hydroxybutyl 4-aryloxybenzoates: Synthesis and Mesomorphic Properties of their H-bonded Complexes with poly(4-vinylpyridine).	593, 93-103	2014
35.	Saira Mumtaz, Rashad Hussain, Abdul Rauf, H. Bokhari, M. Qaiser Fatmi , Michael Oelgemöller, A. M. Qureshi	Medicinal Chemistry Research, ISSN: 1054-2523	Synthesis, Molecular docking studies, and <i>in vitro</i> screening of barbiturates/ thiobarbiturates as antibacterial and cholinesterase inhibitors.	23, 2715-2726	2014
36.	Hira Khalid, Aziz-ur-Rehman, Muhammad Athar Abbasi, Rashad	Turkish Journal of	Synthesis, biological evaluation and molecular docking of N'-(1-	38,	2014

	Hussain, Mohammad Khalid Khan, Muhammad Ashraf, Syeda Abida Ejaz, M. Qaiser Fatmi	Chemistry, ISSN:1300-0527	(phenylsulfonyl) piperidine-4-carbonyl)sulfonohydrazide derivatives.	189-201	
37.	Madiha Tanveer, Hina-ur-Razaq Qureshi, M. Qaiser Fatmi , Tayyaba Yasmin	Pakistan Journal of Botany, ISSN: 0556-3321	<i>In silico</i> prediction of regulatory elements and corresponding protein-DNA interaction in plant promoters.	45, 309-319	2013
38.	Sadia Sultan, M. Iqbal Choudhary, Shamsun Nahar Khan, Urooj Fatima, Muhammad Atif, Rahat Azhar Ali, Atta-ur-Rahman, M. Qaiser Fatmi*	European Journal of Medicinal Chemistry, ISSN: 0223-5234	Fungal Transformation of Cedryl Acetate and α -Glucosidase Inhibition Assay, Quantum Mechanical Calculations and Molecular Docking Studies of its Metabolites.	62, 764-770	2013
39.	Jinfeng Lai, Dimitri Niks, Yachong Wang, Tatiana Domratheva, Thomas Barends, Ryan Olsen, Douglas Elliot, M. Qaiser Fatmi , Chia-en A. Chang, Ilme Schlichting, Michael F. Dunn and Leonard J. Mueller	Journal of the American Chemical Society, ISSN: 0002-7863	X-Ray and NMR crystallography in an enzyme active site: the indoline quinonoid intermediate in tryptophan synthase.	133, 4-7	2011
40.	Khalid Ahmed, Rafia Azmat, Fahim Uddin, M. Qaiser Fatmi	Chinese Journal of Chemistry, ISSN: 1614-7065	Kinetics of reduction of thionine with ribose and structural properties of dye at different pH using DFT methods.	29, 643-649	2011
41.	M. Qaiser Fatmi , Chia-en A. Chang	PLoS Computational Biology, ISSN: 1553-734X	The role of oligomerization and cooperative regulation in protein function: The case of tryptophan synthase.	6, e1000994	2010
42.	Rizi Ai, M. Qaiser Fatmi , Chia-en A. Chang	Journal of Computer-aided Molecular Design, ISSN: 0920-654X	T-Analyst: A program for efficient analysis of protein conformational changes.	24, 819-827	2010
43.	M. Qaiser Fatmi* , Thomas S. Hofer, Bernd M. Rode	Physical Chemistry Chemical Physics, ISSN:1463-9076	The Stability of $[\text{Zn}(\text{NH}_3)_4]^{2+}$ in Water: A Quantum Mechanical/Molecular Mechanical Molecular Dynamics Study	12, 9713-9718	2010
44.	S. Sikander Azam, Zaheer-ul-Haq, M. Qaiser Fatmi*	Journal of Molecular Liquids, ISSN: 0167-7322	Classical and QM/MM MD Simulations of Sodium(I) and Potassium(I) ions in aqueous solution.	153, 95-100	2010
45.	M. Qaiser Fatmi , Rizi Ai, Chia-en A. Chang	Biochemistry, ISSN: 0006-2960	Synergistic Regulation and ligand-induced conformational changes of tryptophan synthase.	48, 9921-9931	2009
46.	M. Qaiser Fatmi , Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode	Journal of Physical Chemistry. B, ISSN:1520-6106	Exploring structure and dynamics of the diaquotriamminezinc(II) complex by QM/MM MD simulation.	112, 5788-5794	2008
47.	M. Qaiser Fatmi , Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode	Journal of Physical Chemistry. B, ISSN:1520-6106	Stability of different zinc(II)-diamine complexes in aqueous solution with respect to structure and dynamics: A QM/MM MD study.	111, 151-158	2007

48.	M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode	Journal of Computational Chemistry, ISSN:0192-8651	Quantum mechanical charge field (QMCF) molecular dynamics simulation of the TiO^{2+} ion in aqueous solution.	28, 1704-1710	2007
49.	M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode	Journal of Physical Chemistry. B, ISSN:1520-6106	Temperature effects on the structural and dynamical properties of the Zn(II)-water complex in aqueous solution: A QM/MM molecular dynamics study.	110, 616-621	2006
50.	M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode	Physical Chemistry Chemical Physics, ISSN:1463-9076	Structure and dynamics of the $[\text{Zn}(\text{NH}_3)(\text{H}_2\text{O})_5]^{2+}$ complex in aqueous solution obtained by an ab initio QM/MM molecular dynamics study.	8, 1675-1681	2006
51.	S. Adnan Ali Shah, Thomas S. Hofer, M. Qaiser Fatmi, Bernhard R. Randolph, Bernd M. Rode	Chemical Physics Letters, ISSN:0009-2614	A QM/MM MD simulation study of hydrated Pd^{2+} .	426, 301-305	2006
52.	Muhammad Iqbal Choudhary, Muhammad Atif, Sarfaraz A. Nawaz, M. Qaiser Fatmi, Atta-ur-Rahman	Natural Product Research, ISSN:1478-6419	The microbiological hydroxylation of levonorgestrel.	20, 1074-1081	2006
53.	M. Qaiser Fatmi, Thomas S. Hofer, Bernhard R. Randolph, Bernd M. Rode	Journal of Chemical Physics, ISSN:0021-9606	An Extended ab initio QM/MM MD approach to structure and dynamics of Zn(II) in aqueous solution.	123, 54514-54521	2005

LIST OF PATENT

#	Name of Authors	Title	Patent by	Organization involved	Patent Application Number	Patent Filing Date	Status
1.	Aneela Yousaf, M. Qaiser Fatmi* , Syed Muhammad Nurulain	A composition comprising Auraptene, for alcohol withdrawal	Government of Pakistan (Intellectual Property Organization)	COMSATS University Islamabad	120/2019	25-02-2019	Under Process

BOOK CHAPTERS

#	Name of Authors	Book Title & Publisher	Title of the Publication	Vol. No. & Page No.	Year Published
1.	Amir Khan, Ali Jan, Muhammad Qaiser Fatmi	Breast Cancer: From Bench to Personalized Medicine. Publisher Springer Singapore	Chapter 12: Therapeutic options in BRCA1-linked breast cancer and systemic approaches	265-280	2022
2.	Ayesha T. Tahir, M. Qaiser Fatmi , Asia Nosheen, Mahrukh Imtiaz, Salma Khan	Essentials of Bioinformatics, Volume III. In Silico Life Sciences: Agriculture. Publisher Springer Nature Switzerland, ISBN 978-3-030-19317-1 (Print) ISBN 978-3-030-19318-8 (eBook)	Chapter 7: Metabolomic Approaches in Plant Research	109-140	2019
3.	Hira Khalid, Aziz-ur-Rehman, M. Athar Abbasi, Rashad Hussain, Abdul Malik, Muhammad Ashraf, M. Qaiser Fatmi (Book Chapter based on Original Research)	Emerging Trends in Chemical Sciences, Publisher Springer, Cham, ISBN978-3-319-60407-7 (Print) ISBN978-3-319-60408-4 (Online)	Synthesis, Spectral Analysis and Biological Evaluation of 5-Substituted 1,3,4-Oxadiazole-2-yl-4-(Piperidin-1-ylsulfonyl)Benzyl Sulfide.	221-238	2018