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or
Village Kuza Durushkheal, Teh. Matta, District Swat, KPK, Pakistan.

Work Philosophy

I believe if it's not coming from deep inside its not going to be impressive & expressive. Whenever I work on a design or a solution I think while in the Client's shoes. Discipline, hard work, consistency and passion are the way to success.

Current Research Interests

Computer-aided development of novel and potent drugs for AIDS, Ulcer, Malaria, Snake Venom, Cancer, Dengue fever and HCV infection.

Current Position

Since May, 2012

Chairman (Acting)

Dept. of Biochemistry, University College of Science (UCS), Shankar, Abdul Wali Khan University, Mardan, Mardan-23200, Pakistan.

Sept. 2011 to Apr. 2012

Assistant Professor

Dept. of Biochemistry, UCS, Shankar, Abdul Wali Khan University, Mardan, Mardan-23200, Pakistan.

Oct. 2010 to Aug. 2011

Assistant Professor

Dept. Of Chemistry, UCS, Shankar, Abdul Wali Khan University Mardan, Mardan-23200, Pakistan.

Courses Taught

1. Computational Medicinal Chemistry.
2. Bioinformatics.
3. Enzymology.
4. Molecular Biology.
5. Biochemistry.

Research Papers

1. **Abdul Wadood**, Muhammad Riaz, Syed Babar Jamal and Masaud Shah. Interactions of ketoamide inhibitors on HCV NS3/4A protease target: Molecular docking study. *Mol. Biol. Rep.* 2013. Accepted.
2. **Abdul Wadood**, Nasir Ahmad, Muhammad Riaz, Sulaiman Shams, Muhammad Ayaz and Javed Anwer. Homology modelling and molecular dynamics study of Candida albicans heat shock protein 21, a potential target protein for anti-fungal development. *Int. J. Sci.* 2013. Accepted
3. Saleha Suleman Khan, Ajmal Khan, Afsar Khan, **Abdul Wadood**, Umer Farooq, Amir Ahmed, Aqib Zahoor, Viqar Uddin Ahmed, Bilge Sener and Nurgum Erdemoglu. Urease inhibitory activity ursane type sulphated saponins from the aerial parts of *Zygophyllum fabago* linn. *Phytomedicine.* 2013. Accepted
4. Masaud Shah, **Abdul Wadood**, Ziaur Rahman and Tayyab Hussain. Interaction and inhibition of dengue envelope glycoprotein with mammalian receptor DC-sign, an in-silico approach. *PLoS One.* 2013, 9, 1-10.
5. **Abdul Wadood** and Zaheer-ul-Haq. In silico identification of novel inhibitors against *Plasmodium falciparum* dihydroorotate dehydrogenase. *J. Mol. Graph. Model.* 2013, 40, 40-47.
6. Sobia Ahsan Halim, Omer Mohamad Abdalla, M. Ahmed Mesaik, **Abdul Wadood**, Zaheer ul-Haq and Maria Kontoyianni. Identification of novel interleukin-2 inhibitors through computational approaches. *Mol. Divers.* 2013, 17, 345-355.
7. Umer Rashid, Iram Batool, **Abdul Wadood**, Ajmal Khan, Zaheer ul-Haq, M. I. Choudhary and Frazana Latif Ansari. Structure based virtual screening-driven identification of monastrol as a potent urease inhibitor. *J. Mol. Graph. Model.* 2013, 43, 47-57.
8. **Abdul Wadood**, Muhammad Riaz, Syed Babar Jamal, Masaud Shah and Muhammad Arif Lodhi. Molecular docking study of P4-benzoxaborole-substituted ligands as inhibitors of HCV NS3/4A protease. *Bioinformation.* 2013, 9, 309-314.

9. Gowhar Ali, Fazal Subhan, **Abdul Wadood**, Ajmal Khan, Nasir Ullah, Nazar Ul Islam and Ikhtiar Khan. Pharmacological evaluation, molecular docking and dynamics simulation studies of salicyl alcohol nitrogen containing derivatives. *Afric. J. Pharm. Pharmacol.* 2013, 7, 585-596.
10. Muhammad Arif Lodhi, Zaheer-ul-Haq, **Abdul Wadood**, Sajid Iqbal, Atta-ur-Rahman and M. Iqbal Choudhary. Three-Dimensional Quantitative Structure Activity Relationship (CoMSIA) Analysis of Bis-coumarine analogues as urease inhibitors. *Med. Chem. Res.* 2013, 22, 498-504.
11. Sahib Gul Afridi, Suleman Shams, Abdul Nasir, Muhammad Junaid, Ashfaq ur Rahman, Muhammad Naeem, Najam Saqib and **Abdul Wadood**. Prevalence of Hepatitis C in Shahbaz Ghari, District Mardan. *Life Sci. J.* 2013. Accepted
12. Suleman Shams, Sahib Gul Afridi, **Abdul Wadood**, Maruh Iqbal, Mehwish Munir, Ummia Shams, Madiha Khan and Shumaila Yousuf. Frequency distribution of ABO, Rh blood group among the students of Abdul Wali Khan University Mardan, Pakistan. *IJAVMS.* 2013. Accepted
13. **Abdul Wadood**, Rabia Sattar, S. Abid Ali and Zaheer-Ul-Haq. A novel pharmacophore model to identify leads for simultaneous inhibition of anti-coagulation and inflammatory activities of snake venom phospholipase A₂. *Chem. Biol. Drug Des.* 2012, 79, 431-441.
14. Syed Sikandar Azam, Reaz Uddin, **Abdul Wadood**. Structure and dynamics of alpha-glucosidase through molecular dynamics simulation. *J. Mol. Liquid.* 2012, 174, 58-62
15. Khalid M. Khan, Muhammad Ali, **Abdul Wadood**, Zaheer-Ul-Haq, M. Khan, M. Arif Lodhi, S. Perveen, M. I. Choudhary and W. Voelter. Molecular modeling-based antioxidant arylidene barbiturates as urease inhibitors. *J. Mol. Graph. Model.* 2011, 30, 153-156.
16. Zaheer-ul-Haq, Reaz Uddin, Lam Kok Wai, **Abdul Wadood** and Nordin Haji Lajis. Docking and 3D-QSAR modeling of cyclin-dependent kinase 5/p25 inhibitors. *J. Mol. Model.* 2011, 17, 1149-1161.
17. Obaid-ur-Rahman Abid, Tariq Mahmood Babar, Farukh Iftakhar Ali, Shahzad Ahmed, **Abdul Wadood**, Nasim Hasan Rama, Reaz Uddin, Zaheer-ul-Haq, Ajmal Khan and M. Iqbal Choudhary. Identification of novel urease inhibitors by high-throughput virtual and in vitro screening. *ACS Med. Chem. Letters.* 2010, 1, 145-149.
18. Khalid M. Khan, **Abdul Wadood**, Muhammad Ali, Zia-Ullah, Zaheer Ul-Haq, M. Arif Lodhi, Momin Khan, Shahnaz Perveen and M. Iqbal Choudhary. Identification of potent urease inhibitors via ligand- and structure-based virtual screening and in vitro assay. *J. Mol. Graph. Model.* 2010, 28, 792-798.
19. Imtiaz Khan, Sajid Ali, Shahid Hameed, Nasim Hasan Rama, Muhammad Tahir Hussain, **Abdul Wadood**, Reaz Uddin, Zaheer Ul-Haq, Ajmal Khan, Sajjad Ali, M. Iqbal Choudhary. Synthesis, antioxidant activities and urease inhibition of some new 1,2,4-triazole and 1,3,4-thiadiazole derivatives.. *Eur. J. Med. Chem.* 2010, 1-8.
20. Zaheer-ul-Haq and **Abdul Wadood**. Prediction of binding affinities for hydroxamic acid derivatives as urease inhibitors by molecular docking and 3D-QSAR. *Lett. Drug. Des. Discov.* 2009, 6, 93-100.
21. Farzana Latif Ansari, **Abdul Wadood**, Ahsan Ullah, Fatima Iftikhar and Zaheer-ul-Haq. "In silico studies of urease inhibitors to explore ligand-enzyme interaction". *J. Enz. Inhib. Med. Chem.* 2009, 24 (1) 151-156.
22. Zaheer-ul-Haq, **Abdul Wadood** and Reaz uddin. "CoMFA and CoMSIA 3D-QSAR analysis on hydroxamic acid derivatives as urease". *J. Enz. Inhib. Med. Chem.* 2009, 24 (1) 272-278.
23. **Abdul Wadood** and Syed Babar. Computational analysis of Benzofuran-2-carboxylic acid as potent Pim-1 kinase inhibitor. Submitted
24. **Abdul Wadood**, Syed Babar Jamal and Muhammad Riaz. Analysis of the Pim-1 kinase inhibitory activity of 3H-Benzo(4,5)thieno(3,2-d)pyrimidin-4-one derivatives based on their molecular features: a computational study. *J. Saudi. Chem. Soc.* submitted
25. **Abdul Wadood**, Muhammad Riaz and Zaheer-ul-Haq. Identification and evaluation of leads for the simultaneous inhibition of protease and helicase activities of HCV NS3/4A protease using complex based pharmacophore mapping and virtual screening. *J. Chem. Info. Model.* submitted

Academic

- 2010 - :** **Ph.D. in Chemistry**
Computational Medicinal Chemistry Laboratory, H. E. J. Research Institute of Chemistry, University of Karachi, Karachi-75270, Pakistan.
- 2007 - :** **International GRE (ETS) in Biochemistry, Cell Biology and Molecular biology**
Total Score: 560, Percentile: 65.
- 2005 - :** **Ph.D. Course Work**
Six months M. Phil./Ph.D. Course Work has been completed in the subjects
Physical Method of Isolation & Structural Elucidation, Protein Biochemistry, Enzymology and Biochemistry.
H. E. J. Research Institute of Chemistry, University of Karachi, Karachi-75270, Pakistan.
- 2004 - :** **M.Sc (Biochemistry) Grade: 2nd Division.**
Deptt. Of Biochemistry, University of Karachi, Karachi-75270, Pakistan.
- 1999 - :** **B.Sc (Biochemistry, Microbiology and Botany) Grade: 1st Division**
University of Karachi, Karachi, Pakistan.
- 1995 - :** **Higher Secondary School Certificate (HSCC) Grade: 1st Division**
Board of Intermediate Education Karachi, Pakistan.

WORKSHOPS / CONFERENCES / INTERNSHIPS

- 8-11th Jan. 2005: Poster Presentation in International Conference on Protein Structure Determination, ICCBS. University of Karachi, Pakistan.
- 6-9th Jan. 2006: Poster Presentation in 10th International Symposium on Natural Product Chemistry, ICCBS. University of Karachi, Pakistan.
- 26-28th June 2006: Workshop on "Computational Chemistry and its Applications", ICBCS. University of Karachi, Pakistan.
- 17-20th Jan. 2007: Poster Presentation in 1st International Symposium-cum-Training Course on Molecular Medicine and Drug Research (MMDR), Dr. Panjawani Centre for Molecular Medicine and Drug Research (PCMD), ICCBS, University of Karachi, Pakistan.
- Oct.29-Nov.01/2008: Poster Presentation in 11th International Symposium on Natural Product Chemistry, ICCBS. University of Karachi, Pakistan.
- 12-15th Jan. 2009: Poster Presentation in 2nd International Symposium-cum-Training Course on Molecular Medicine and Drug Research (MMDR-2), Dr. Panjawani Centre for Molecular Medicine and Drug Research (PCMD), ICCBS. University of Karachi, Pakistan.
- 14-15th May 2012: Oral presentation in Two Days Workshop on Bioinformatics in Medicine, Institute of Biomedical Sciences, Khyber Medical University, Peshawar, Pakistan.

Supervision

Master Thesis Research Students	09
M. Phil. Research Students	05
Ph. D. Research Studnts	Nil

Research Porject Awarded by different funding agencies **03**

Areas of Exertise

- Pharmacophore Modeling.
- Structure-based and ligand-based Virtual Screening.
- Molecular Docking.
- Molecular Dynamics simulation
- Exploring Protein Ligand interactions.
- 3D-QSAR Studies.
- Protein structure and function prediction.
- Homology Modeling.
- Structure Optimization.
- High-throughput screening using 96-well plate.

Computational Chemistry Skills

- Sybyl, MOE, Gromacs, LigandScout, GOLD, AutoDock, Dock, MOE-Dock, FRID.
- Modeller, Gausview, VMD, CHIMERA, Molden, Marvin Sketch, PYMOL, RASMOL,
- SILVER, LIGPLOT.

References

1. Asst. Prof. Dr. Zaheer-ul-Haq

Dr. Panjwani Center for Molecular Medicine and Drug Research, University of Karachi, Karachi, Pakistan.

zaheer_qasmi@hotmail.com, zaheer.qasmi@iccs.edu

2. Asst. Prof. Dr. Reaz Uddin

Dr. Panjwani Center for Molecular Medicine and Drug Research, University of Karachi, Karachi, Pakistan.

riaasuddin@yahoo.com

3. Asst. Prof. Dr. Momin Khan

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