

Dr. Abdul Wadood

Mobile Number: +92 345-2683291

Email Address: awdood@awkum.edu.pk , awadood2001@yahoo.com

Residence: Village Kuza Durushkheal, Teh. Matta, District Swat, KPK, Pakistan.

Work Philosophy

I believe if it's not coming from deep inside it's 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 Diabetes, Cancer, Ulcer, Malaria, Alzheimer, Dengue fever, HCV and HIV infection.

Current Position

June, 2017 to date

Tenured Associate Professor

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

June, 2011 to May, 2017

Assistant Professor (TTS)

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

October, 2010 to May 2011

Assistant Professor (IPFP)

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

September, 2014 to Feb. 2015

Six months Postdoctoral study in the research group of Prof. Dr. Richard Bryce, University of Manchester, UK.

Academics

2010

Ph.D. in Chemistry,

Computational Medicinal Chemistry Laboratory, H. E. J. Research Institute of Chemistry, University of Karachi, Karachi-75270, Pakistan.

2004

M.Sc(Biochemistry), University of Karachi

1999

B.Sc(Biochemistry, Microbiology and Botany) University of Karachi

1995

FSC, Board of Intermediate Education Karachi, Pakistan

1992

SCC, BISE, SaiduSherif Swat, Pakistan

Area of Expertise

Pharmacophore Modeling, Subtractive genome analyses, 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.

Software Expertise

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

Supervision

Master Thesis Research Students	20
M. Phil. Research Students	08
Ph. D. Research Students	Nil

Undersupervision

M. Phil student	08
Ph. D. Student	03

Research Projects

1. No. 20-3479/NRPU/R&D/HEC/2017 under the title: Application of NGS and Bioinformatics in Molecular Diagnosis and Clinical Practice of Dermatology.
Rs. 3.0 million awarded by Higher Education Commission of Pakistan (HEC).
2. No. 20-2781/NRPU/R&D/HEC/2015 under the title: *Computational and Theoretical Studies of HCV NS3/4A Protease* of Rs. 3.5 Million Awarded by Higher Education of Pakistan (HEC).
3. Start up Research Grant under the title: Structure-Based Approach to Design Antiparasitics: Inhibition of Pyrimidine Biosynthesis Enzymes in Malaria.
Rs. 0.5 million awarded by Higher Education Commission of Pakistan (HEC).

Research Awards

1. Research Productive Award by Pakistan Council for Science and Technology for the year 2017.
2. Research Productive Award by Pakistan Council for Science and Technology for the year 2016.
3. Research Productive Award by Pakistan Council for Science and Technology for the year 2015.
4. Best Researcher Award by Abdul Wali Khan University Mardan, Pakistan for the year 2014.
5. Best Researcher Award by Abdul Wali Khan University Mardan, Pakistan for the year 2013.

List of Publications

2019

1. Kanwal, Khalid Mohammed Khan, UzmaSalar, Saira Afzal, **Abdul Wadood**, Muhammad Taha, S. Perveen, Huma Khan, Joanna Lecka, Jean Sevigny, Jamshed Iqbal. Schiff bases of tryptamine as potent inhibitors of nucleoside triphosphate diphosphohydrolases (NTPDases): Structure-activity relationship. *Bioorg. Chem.* 2019, 82, 253-266.
2. M. Ayaz, A. Sadiq, **A. Wadood**, M. Junaid, F. Ullah, N. Z. Khan. Cytotoxicity and molecular docking studies on phytosterols isolated from *Polygonum hydropiper* L. *Steroids*, 2019, 30-35.
3. N. Naz, M. Sirajuddin, A. Haider, S. M. Abbas, S. Ali, **A. Wadood**, M. Ghufuran, G. Rehman and B. Mirza. Synthesis, characterization, Biological screening and molecular docking study of organotin(IV) derivatives of 2,4-dichlorophenoxyacetic acid. *J. Mol. Struct.*, 2019, 662-671.
4. R. Uddin, F. Masood, S. S. Azam, **A. Wadood**. Identification of putative non-host essential genes and novel drug targets against *Acinetobacter baumannii* by in silico comparative genome analysis. *Microb. Pathog.*, 2019, accepted.
5. Ghulam Mohiuddin, Khalid Mohammed Khan, UzmaSalar, Kanwal, Muhammad Arif Lodhi, **Abdul Wadood**, Muhammad Riaz, Shahnaz Perveen. Biology-oriented drug synthesis (BIODS), in vitro urease inhibitory activity, and in silico study of S-naproxen derivatives. *Bioorg. Chem.* 2019, 83, 29-46.

2018

6. **Abdul Wadood**, Alam Jamal, Muhammad Riaz, Ajmal Khan, Reaz Uddin, Musharrf Jelani and Syed Sikander Azam. Subtractive genome analysis for in silico identification and characterization of novel drug targets in *Seteptococcus pneumonia* strain JJA. *Microb. Pathog.* **2018**, 115, 194-198.
7. **Abdul Wadood**, Mehreen Ghufuran, Ajmal Khan, Syed Sikander Azam, Musharraf Jelani and Reaz Uddin. Selective glycosidase inhibitors: A patent review (2012-present). *Int. J. Biol. Macromol.* **2018**, 111, 82-91.
8. Hanif Ahmad, Shujaat Ahmad, Mumtaz Ali, Abdul Latif, Syed Adnan Ali Shah, HumeraNaz, Najeeb ur Rahman, Farzana Shaheen, **Abdul Wadood**, Hidayat Ullah Khan and Manzoor Ahmad. Norditerpenoid alkaloids of *Delphinium denudatum* as cholinesterase inhibitors. *Bioorg. Chem.* 2018, 78, 427-435.
9. Sahar Yousuf, Khalid Mohammed Khan, UzmaSalar, Sridevi Chigurupati, Munira Taj Muhammad, **Abdul Wadood**, MahaAldubayan, Venugopal Vijayan, Muhammad Riaz, Shahnaz

- Perveen. 2'-Aryl and 4'-arylidene substituted pyrazolones: As potential α -amylase inhibitors. Eur. J. Med. Chem. 2018, 159, 47-58.
10. Basharat Ali, Khalid Mohammad Khan, Arshia, Kanwal, Shafaqat Hussain, Safdar Hussain, Muhammad Ashraf, Muhammad Riaz, **Abdul Wadood** and Shahnaz Perveen. Synthesis of nicotinic/isonicotinic thiosemicarbazides: In vitro urease inhibitory activities and molecular docking studies. Bioorg. Chem. 2018, 79, 34-45.
 11. Najeeb Ur Rehman, Ajmal Khan, Ahmed Al-Harrasi, H. Hussain, **Abdul Wadood**, Muhammad Riaz and Zahra Al-Abri. New α -glucosidase inhibitors from the resins of Boswellia species with structure-glucosidase activity and molecular docking studies. Bioorg. Chem. 2018, 79, 27-33.
 12. Zia Ud Din, MA Trapp, LSD Medeiros, DL Bidoia, FP Gracia, F Peron, CV Nakamura, IC Rodriguez, **Abdul Wadood**, ER Filho. Symmetrical and unsymmetrical 2,5-diarylidene cyclohexanones as anti-parasitic compounds. Eur. J. Med. Chem. 2018, 155, 596-608.
 13. Tareq Abu-Izneid, Abdul Rauf, Syed Uzair Ali Shah, **Abdul Wadood**, Mohammed I. S. Abdelhady, Priymenko Nathalie, Domange Celine, Nashwa Mansour and Seema Patel. BioMed Res. Int. 2018.
 14. Muhammad Ali, K. M. Khan, Uzma Salar, M. Ashraf, Muhammad Taha, **Abdul Wadood**, Sujhla Hamid, Muhammad Riaz, Basharat Ali, Shahbaz Shamim, Farman Ali and Shahnaz Perveen. Synthesis, in vitro α -glucosidase inhibitory activity, and in silico study of (E)-thiosemicarbazones and (E)-2-(2-(arylmethylene)hydrazinyl)-4-arylthiazole derivatives. Mol. Div. 2018.
 15. Najeeb Ur Rehman, Raed MM Abed, Hidayat Hussain, Hussain Yar Khan, Ajmal Khan, Abdul L. Khan, Majid Ali, Abdullah Al-Nasri, Khalid Al-Harrasi, Ahmed N. Al-Rawahi, **Abdul Wadood**, Ahmed Al-Rawahi, Ahmed Al-Harrasi. Ant-proliferative potential of cyclotrapeptides from Bacillus velezensis RA5401 and their molecular docking on G-Protein Coupled. Microbial. Pathog. 2018, 123, 419-425.
 16. Muhammad Taha and **Abdul Wadood**. Synthesis and molecular docking study of piperazine derivatives as potent urease inhibitors. Bioorg. Chem. 2018, 78, 411-417.
 17. Rehman AU, Rehman MU, Tahir KM, Saud S, Liu H, Song D, Sultana P, **Wadood A**, Chen HF. The Landscape of protein tyrosine phosphatase (Shp2) and cancer. Curr. Pharm. Des. 2018.
 18. M Alam, A Khan, **A Wadood**, S Bashir, A Aman, U Farooq, FA Khan, F Mabood, J Hussain, Samiullah and A Al-Harrasi. Bioassay-guided isolation of urease inhibitors from Ferula narthex. Bioss. South African J. Botany. 2018.
 19. Momin Khan, Aftab Alam, Khalid Muhammad Khan, Uzma Salar, S. Chigurupati, **Abdul Wadood**, Farman Ali, Jahidul Islam Mohammad, Muhammad Riaz and Shahnaz Perveen.

- Flurbiprofen derivative as novel α -amylase inhibitors: Biology-oriented drug synthesis (BODS), In vitro and in silico evaluation. *Bioorg. Chem.* 2018, 81, 157-167.
20. S. F. Ahmad, Ibrar Khan, **Abdul Wadood**, Sadiq Azam, Noor Rehman, Muhammad Waqas, Kashif Bashir and Asaf Ali Khan. Pathogen Constancy, harbinger of nosocomial infection cum identification of resistant genes and drug designing. *Comput. Biol. Drug Des.* 2018, 74, 347-359.
 21. A. T. Bale, K. M. Khan, Uzma Salar, S. Chigurupati, T. Fasina, Farman Ali, Kanwal, **Abdul Wadood**, Muhammad Taha, S. S. Nanda, Mehreen Ghufraan and Shahnaz Perveen. *Bioorg. Chem.* 2018, 79, 179-189.
 22. M. T. Javed, Fazal Rahim, Muhammad Taha, Mohsan Nawaz, **Abdul Wadood**, Muhammad Ali, Ashik Mosaddik, Syed Adnan Ali Shah and Rai Khalid Farooq. Synthesis SAR elucidations and molecular docking study of newly designed isatin based oxadiazole analogs as potent inhibitors of thymidine phosphorylase. *Bioorg. Chem.* 2018, 79, 323-333.
 23. Ahmad S, Navid A, Akhtar AS, Azam SS, **Wadood A** and Perez-Sanchez. Subtractive genomics, molecular docking and molecular dynamics simulation revealed LpxC as potential drug target against multi-drug resistant *Klebsiella pneumoniae*. *Interdiscip. Sci.* 2018.
 24. Reaz Uddin, Quratulain Nehal Siddiqui, Syed Sikander Azam, Bibi Saima and **Abdul Wadood**. *Eur. J. Pharm. Sci.* 2018, 114, 13-23.
 25. Fazle Subhan, Sobia Aslam, Zifeng Yan, Zhen liu, UJ Etim, **Abdul Wadood** and Rooh Ullah. Confinement of mesopores within ZSM-5 and functionalization with Ni NPs for deep desulfurization. *Chem. Eng. J.* 2018, 354, 706-715.
 26. Khan M. Khan S, Ul Mulk A, Ur Rahman A, **Wadood A**, Shams S, Ashraf M, Rahman J, Hameed A, Hussain Z, Khan A, Zaman K, Khan KM and Perveen S. Synthesis molecular modeling and biological evaluation of 5-arylidine-N,N-diethylthiobarbiturates as potential α -glucosidase inhibitors. *Med. Chem.* 2018.
 27. Salar U, Khan KM, Chigurupati S, Syed S, Vijayabalan S, **Wadood A**, Riaz M. Ghufraan M and Perveen S. New hybrid scaffolds based on hydrazinylthiazole substituted coumarin; As novel leads of dual potential; In vitro α -amylase inhibitory and antioxidant (DPPH and ABTS radical Scavenging) activities. *Med. Chem.* 2018.
 28. Niaz Muhammad, Naseer Ali Shah, Saqib Ali, **Abdul Wadood**, Mehreen Ghufraan, Muhammad Rahsid Khan, Pakiza Siddiq, Shaikat Shujah and Auke Meetsma. Antimicrobial efficiency of diorganotin (IV) bis-[3-(4-chlorophenyl)-2-methylacrylate]. *J. Coord. Chem.* 2018.
 29. SK Avula, A Khan, NU Rehman, MU Anwar, Z Al-Abri, **Abdul Wadood**, M Riaz, R Csuk, A Al-Harrasi. Synthesis of 1H-1,2,3-triazole derivatives as new α -glucosidase inhibitors and their molecular docking studies. *Bioorg. Chem.* 2018, 81, 98-106.

30. Basharat Ali, Khalid Mohammad Khan, UzmaSalar, Kanwal, Safdar Hussain, M. Ashraf, Muhammad Riaz, **Abdul Wadood**, M. Taha and S.Perveen. *Bioorg. Chem.* 2018, 79, 363-371.
31. Syed Sikander Azam, Sajjad Ahmad, AfifaNavid, Noor Ul Ain Sahid, Iqra Ahmad and **Abdul Wadood**. Implication of sequence conservation patterns of serpin B family leading to structural and functional importance. *Gene Reports.* 2018, 12, 30-38.
32. Imad Uddin, Muhammad Taha, Fazal Rahim and **Abdul Wadood**. Synthesis and molecular docking study of piperazine derivatives as potent inhibitors of thymidine phosphorylase. *Bioorg. Chem.* 2018, 78, 324-331.
33. Hayat ullah, Fazal Rahim, Muhammad Taha, Imad Uddin, **Abdul Wadood**, S. Adnan Ali Shah, R. K. Farooq, Mohsan Nawaz, Zainul Wahab, Khalid Muhammad Khan. Synthesis, molecular docking study and in vitro thymidine phosphorylase inhibitory potential of oxadiazole derivatives. *Bioorg. Chem.* 2018, 78, 58-67.
34. M. Tariq Javed, Fazal Rahim, M. Taha, Haseeb Ur Rehman, M. Nawaz, **Abdul Wadood**, Syahrul Imran, Imad Uddin, Ashik Musaddik, K. M. Khan. Synthesis, in vitro α -glucosidase inhibitory potential and molecular docking study of thiadiazoleanalogs. *Bioorg. Chem.* 2018, 78, 201-209.
35. A. AkinsolaAdegboye, Khalid Muhammad Khan, UzmaSalar, S. Adeyinka Aboaba, Kanwal, S. Chigurupati, Itrat Fatima, Mohammad Taha, **Abdul Wadood**, J. Islam Mohammad, Huma Khan, Shahnaz Perveen. 2-Aryl benzimidazoles: Synthesis, In vitro α -amylase inhibitory activity, and molecular docking study. *Eur. J. Med. Chem.* 2018, 150, 248-260.
36. Muhammad Taha, Syahrul Imran, Fazal Rahim, **Abdul Wadood**, K. M. Khan. Oxindole based oxadiazole hybrid analogs: Novel α -glucosidase inhibitors. *Bioorg. Chem.* 2018, 76, 273-280.
37. Niaz Muhammad, Muhammad Ikram, **Abdul Wadood**, Sadia Rehman, Shaukat Shujah, Erum, MehreenGhufran, Shahnaz Rahim, Muzamil Shah, Carola Schulzke. Synthesis, crystal structure, DNA binding and molecular docking studies of zinc (II) carboxylates. *Spectrochem. Acta Part A. Mol. Biomol. Spect.* 2018, 190, 368-377.
38. UzmaSalar, Khalid M Khan, Fakhri MI, Hussain S, Tauseef S, Ameer S, **Abdul Wadood**, Khan H and Perveen S. 1,1'-Carbonyldiimidazole (CDI) mediated facile synthesis, structural characterization, antimicrobial activity and in-silico studies of coumarin-3-carboxamide derivatives. *Med. Chem.* 2018, 14, 86-101.

2017

39. **Abdul Wadood**, Mehreen Ghufuran, Asifullah Khan, Syed Sikander Azam, Reaz Uddin, Muhammad Waqas and Shoib Saleem. The methicillin-resistant *S. epidermitis* strain RP62A genome mining for potential Novel drug target identification. *Gene Reports*, 2017, 8, 88-93.
40. **Abdul Wadood**, Mehreen Ghufuran, Umer Rashid, Syed Fahad Hassan. In silico identification of promiscuous scaffolds as potential inhibitors of 1-deoxy-d-xylulose 5-phosphate reductoisomerase for treatment of *Falciparum malaria*. *Pharm. Biol.* 2017, 55, 19-32.
41. **Abdul Wadood**, Aamir Mehmood, Huma Khan, Muhammad Ilyas, Ayaz Ahmad, Mohammad Alarjah and Tareq Abu-Izneid. Epitope based drug design for dengue virus envelope protein: A computational approach. *Comput. Biol. Chem.* 2017, 71, 152-160.
42. Hanif Ahmed, Shujjat Ahmed, Syed Adnan A. Shah, Abdul Latif, M. Ali, F. A. Khan, Muhammad Nawaz Tahir, Farzana Shaheen, **Abdul Wadood** and M. Ahmad. Antioxidant and anticholinesterase potential of diterpenoid alkaloids from *Acontumheterophyllum*. *Bioorg. Med. Chem.* 2017, 25, 3368-3376.
43. Bilquees Bano, Arshia, Khalid M. Khan, Kanwal, Bibi Fatima, M. Taha, N. Hidiyani Ismail, **Abdul Wadood**, Mehreen Ghufuran, Shahnaz Perveen. Synthesis, in vitro glucuronidase inhibitory potential and molecular docking studies of quinolines. *Eur. J. Med. Chem.* 2017, 139, 849-864.
44. **Abdul Wadood**, Huma Khan, Mehreen Ghufuran, Hammad Hassan, Sulaiman Shams, Ajmal Khan, Syed Sikander Azam and Reaz Uddin. Structure-based development of new and potent inhibitors of PIM kinases: A computational study. *Pak. Chem. Soc.* 2017, 39, 132-141.
45. Maria A. Khan, K. Javed, **A. Wadood**, A. Jamal, F. Batool, S. Fazal-ur-Rehman, Fatima Z. Basha, M. I. Choudhary. In vitro α -glucosidase inhibition by non-sugar based triazoles of diabenzoazepine, their structure-activity relationship, and molecular docking. *Med. Chem.* 2017, 13.
46. Momin Khan, Muhammad Yousaf, **Abdul Wadood**, Zahid Hussain, Muhammad Naeem, Khalid Muhammad Khan, Shahnaz Perveen. 2-indolinone derivatives as potent urease inhibitors. *Lett. Drug Des. Discov.* 2017, 14.
47. Uzma Salar, Khalid Muhammad Khan, S. Chigurupati, Muhammad Taha, **Abdul Wadood**, Shantini Vijayabalan, Mehreen Ghufuran and Shahnaz Perveen. New hybrid hydrazinylthiazole substituted chromones: As potential α -amylase inhibitors and radical (DPPH & ABTS) scavengers. *Scientific Reports*. 2017, 7, 1680.

48. UzmaSalar, Khalid Mohammed Khan, Muhammad Taha, Nor Hadiani Ismail, Basharat Ali, Qurat-ul-Ain, Shahnaz Perveen, MehreenGhufran, **Abdul Wadood**: Biology-oriented drug synthesis (BIODS): In vitro β -glucuronidase inhibitory and in silico studies on 2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl aryl carboxylate derivatives. *Eur. J. Med. Chem.* 2017, 125, 1289-1299.
49. Muhammad Taha, Nor Hadiani Ismail, H. MohdZaki, **Abdul Wadood**, E. H. Anouar, S. Imran, B. M. Yamin, Muhammad Ali and K. M. Khan. 3, 4-Dimethoxybenzohydrazide derivatives as antiulcer: Molecular modelling and density functional studies. *Bioorg. Chem.* 2017, 75, 235-241.
50. Muhammad Ayaz, Muhammad Junaid, Farhat Ullah, Fazal Subhan, Abdul Sadiq, Gowhar Ali, Muhammad Owais, Muhammad Shahid, Ashfaq Ahmad, **Abdul Wadood**, Mohamed El-Shazly, Nisar Ahmad and Sajjad Ahmad. Anti Alzheimer's studies on β -sitosterol isolated from *Polygonum hydropiper* L. *Frontier in Pharmacology.* 2017, 8.
51. Sobia Ahsan Halim, Shanaz Khan, Ajmal Khan, **Abdul Wadood**, Fazal Maboob, Javid Hussain and Ahmed Al-Harrasi. Targeting dengue virus NS-3 helicase by ligand based pharmacophore modelling and structure-based virtual screening. *Frontier in Chemistry.* 2017, 5.
52. Tanzila Arshad, Khalid Mohammed Khan, Najma Rasool, UzmaSalar, Shafqat Hussain, Humna Asghar, Mohammed Ashraf, **Abdul Wadood**, Muhammad Riaz, Shahnaz Perveen, Muhammad Taha, Nor Hadiani Ismail: *5-Bromo-2-Aryl benzimidazole Derivatives as Non-Cytotoxic Potential Dual Inhibitors of α -Glucosidase and Urease Enzymes.* *Bioorg. Chem.* 2017, 72, 21-31.
53. Farman Ali, Khalid Muhammad Khan, UzmaSalar, Mohammad Taha, Nor Hadiani Ismail, **Abdul Wadood**, Muhammad Riaz and Shahnaz Perveen. Hydrazinylarylthiazole based pyridine scaffolds: Synthesis, structural characterization, in vitro α -glucosidase inhibitory activity, and in silico studies. *Eur. J. Med. Chem.* 2017, 138, 255-272.
54. Reaz Uddin, SyedaSumayya, Syed Sikander Azam, **Abdul Wadood**, Syed TariqueMoin. Identification of Histone Deacetylase (HDAC) as a drug target against MRSA via interolog method of protein-protein interaction prediction. *Eur. J. Pharm. Sci.* 2017, 106, 198-211.
55. Assem Barakat, Abdullah Mohammad Al-Majid, Saied M. Soliman, Mohammad Shahidul Islam, Hussain Mansur Ghawas, Sammer Yousuf, M. Iqbal Choudhary, **Abdul Wadood**. *Monoalkylated barbiturate derivatives: X-ray crystal structure, theoretical studies, and biological activities.* *J. Mol. Struct.* 2017, 1141, 624-633.

56. Muhammad Taha, Syed Adnan Ali Shah, Muhammad Afifi, ManarZulkeflee, Sadia Sultan, **Abdul Wadood**, Fazal Rahim, Nor Hadiani Ismail: Morpholine hydrazone scaffold: Synthesis, anticancer activity and docking studies. *Chinese Chem. Lett.* 2017, 28, 607-611.
57. Asifullah Khan, Mehwish Munir, Sara Aiman, **Abdul Wadood**, Arif-ullah Khan: *The in silico identification of small molecules for protein-protein interaction inhibition in AKAP-Lbc-RhoAsignaling complex.* *Comput. Biol. and Chem.* 2017, 67, 84-91.
58. KaoutherMajouli, Mohamed Ali Mahjoub, Fazal Rahim, Assia Hamdi, **Abdul Wadood**, Malek BesbesHlila, AbderraoufKenani: *Biological properties of Hertiacheirifolia L. flower extracts and effect of the nopol on α -glucosidase.* *Int. J. Biol. Macromol.* 2017, 95, 757-761.
59. Mohammad Shoib, MehreenGhias, Niaz Ali, **Abdul Wadood**, Syed. Wadood Ali Shah, Ismail Shah, Shafiullah, MehreenGhufran and Mehboob ur Rehman. Synthesis docking studies and pharmacological activities of a synthetic flavonols. *Chiang Mai J. Sci.* 2017, 44(X), 1-11.

2016

60. UzmaSalar, Khalid Mohammed Khan, Shazia Syed, Muhammad Taha, Farman Ali, Nor Hadiani Ismail, Shahnaz Perveen, **Abdul Wadood**, MehreenGhufran: Synthesis, In Vitro β -Glucuronidase Inhibitory Activity and In Silico Studies of Novel (E)-4-Aryl-2-(2-(pyren-1-ylmethylene)hydrazinyl)thiazoles. *Bioorg. Chem.* 2016, 70, 199-209.
61. Nik Khairunissa Nik Abdullah Zawawi, Muhammad Taha, NorizanAhmat, Nor Hadiani Ismail, **Abdul Wadood**, Fazal Rahim: Synthesis, Molecular Docking Studies of Hybrid Benzimidazole As α -Glucosidase Inhibitor. *Bioorg. Chem.* 2016, 70, 184-191.
62. Mahboob Alam, Ajmal Khan, **Abdul Wadood**, Ayesha Khan, Shumaila Bashir, Akhtar Aman, Abdul Khaliq Jan, Abdur Rauf, Bashir Ahmad, Abdur Rahman Khan, Umar Farooq: Corrigendum: Bioassay-Guided Isolation of Sesquiterpene Coumarins from *Ferula narthex* Bioss: A New Anticancer Agent. *Frontiers in Pharmacology.* 2016, 7.
63. Assem Barakat, Bandar M. Al-Qahtani, Abdullah M. Al-Majid, M. Ali Mohammed Rafi Shaik, Mohamed H.M. Al-Agamy, **Abdul Wadood**. Synthesis, characterization, antimicrobial activity and molecular docking studies of combined pyrazol-barbituric acid pharmacophores. *Trop. J. Pharmaceut. Res.* 2016, 15, 2197-2207.
64. Shujjat Ahmad, Hanif Ahmad, Hidayat Ullah Khan, Adnan Shahzad, Ezzat Khan, Syed Adnan Ali Shah, Mumtaz Ali, Abdul Wadood, MehreenGhufran, HumeraNaz and Manzoor Ahmad.

- Crystal structure, phytochemical study and enzyme inhibition activity of Ajaconine and Delectinine. *J. Mol. Struct.* 2016, 1123, 441-448.
65. Sundus Iqbal, Amen Shamim, Syed Sikander Azam, **Abdul Wadood**: Identification of potent inhibitors for chromodomain-helicase- DNA-binding protein 1-like through molecular docking studies. *Med. Chem. Res.* 2016, 25, 2924-2939.
66. Khalid Mohammed Khan, SairaQurban, UzmaSalar, Muhammad Taha, Shafqat Hussain, Shahnaz Perveen, Abdul Hameed, Nor Hadiani Ismail, Muhammad Riaz, **Abdul Wadood**: *Synthesis, In Vitro α -Glucosidase Inhibitory Activity and Molecular Docking Studies of New Thiazole Derivatives.* *Bioorg. Chem.* 2016, 68, 245-258.
67. Mueed Ur Rahman, Hao Liu, Haifeng Chen, **Abdul Wadood**: Allosteric Mechanism of Cyclopropylindolobenzazepine Inhibitors for HCV NS5B Rdrp via Dynamics Correlation Network Analysis. *Mol. BioSyst.* 2016, 12, 3280-3293.
68. Muhammad Taha, Nor Hadiani Ismail, Syahrul Imran, Fazal Rahim, **Abdul Wadood**, Laode Muhammad Ramadhan Al Muqarrabun, Khalid Mohammed Khan, MehreenGhufran, Muhammad Ali: *In Silico Binding Analysis and SAR Elucidations of Newly Designed Benzopyrazine Analogues as Potent Inhibitors of Thymidine Phosphorylase.* *Bioorg. Chem.* 2016, 68, 80-89.
69. Tanzila Arshad, Khalid Mohammed Khan, Najma Rasool, UzmaSalar, Shafqat Hussain, Tehreem Tahir, Mohammed Ashraf, **Abdul Wadood**, Muhammad Riaz, Shahnaz Perveen, Muhammad Taha, Nor Hadiani Ismail: *Syntheses, in vitro evaluation and molecular docking studies of 5-bromo-2-aryl benzimidazoles as α -glucosidase inhibitors.* *Med. Chem. Res.* 2016, 25, 2058-2069.
70. Muhammad Taha, N. H. Ismail, Syahrul Imran, Fazal Rahim, **Abdul Wadood**, Huma Khan, Hayat Ullah, U. Salar, K. M. Khan: *Synthesis, β -Glucuronidase Inhibition and Molecular Docking Studies of Hybrid Bisindole-ThiosemicarbazidesAnalog.* *Bioorg. Chem.* 2016, 68, 56-63.
71. Fazal Rahim, Hayat Ullah, Muhammad Taha, **Abdul Wadood**, Muhammad Tariq Javed, Wajid Rehman, Mohsan Nawaz, Muhammad Ashraf, Muhammad Ali, Muhammad Sajid, Farman Ali, Muhammad Naseem Khan, Khalid Mohammed Khan: *Synthesis and in vitro Acetylcholinesterase and Butyrylcholinesterase Inhibitory Potential of Hydrazide based Schiff Bases.* *Bioorg. Chem.* 2016, 68, 30-40.
72. Muhammad Taha, Nor HadianiImmail, Syahrul Imran, **Abdul Wadood**, Fazal Rahim, Laode Muhammad Ramadhan Al Muqarrabin, HamizahMohdZaki, NorizanAhmat, Abdul Nasir, Fahad

- Khan: Synthesis of Novel Disulfide and Sulfone hybrid Scaffolds as Potent β -glucuronidase Inhibitor. *Bioorg. Chem.* 2016, 68, 15-22.
73. Uzma Salar, M. Taha, Khalid Mohammed Khan, N. H. Ismail, S. Imran, Shahnaz Perveen, Sahib Gul, **Abdul Wadood**: Syntheses of new 3-thiazolyl coumarin derivatives, in vitro α -glucosidase inhibitory activity, and molecular modeling studies. *Eur. J. Med. Chem.* 2016, 122, 196-204.
74. Farman Ali, Khalid Mohammed Khan, Uzma Salar, Sarosh Iqbal, Muhammad Taha, Nor Hadiani Ismail, Shahnaz Perveen, **Abdul Wadood**, Mehreen Ghufuran, Basharat Ali: *Dihydropyrimidones: As Novel Class of β -Glucuronidase Inhibitors*. *Bioorg. Med. Chem.* 2016, 24, 3624-3635.
75. Irfan Ullah, Jamshaid Ali Khan, Achyut Adhikari, Ajmal Khan, Peer Abdul Hannan, **Abdul Wadood** and, Umar Farooq: Bioassay- guided Isolation of New Urease Inhibitory Constituents from *Monotheca buxifolia* (Falc.) Fruit and Their Molecular Docking Studies. *Records of Nat. Product.* 2016, 10, 744-749.
76. Muhammad Taha, N. H. Ismail, S. Imran, **Abdul Wadood**, Fazal Rahim, S. M. Saad, Khalid Mohammed Khan, Abdul Nasir: Synthesis, Molecular Docking and α -Glucosidase Inhibition of 5-Aryl-2-(6'-nitrobenzofuran-2'-yl)-1,3,4-oxadiazoles. *Bioorg. Chem.* 2016, 66, 117-123.
77. Muhammad Taha, Nor Hadiani Ismail, Syahrul Imran, **Abdul Wadood**, Fazal Rahim, Khalid Muhammad Khan, Muhammad Riaz: Hybrid Benzothiazole analogs as Antiurease Agent: Synthesis and Molecular Docking Studies. *Bioorg. Chem.* 2016, 66, 80-87.
78. Muhammad Taha, Nor Hadiani Ismail, Syahrul Imran, **Abdul Wadood**, Muhammad Ali, Fazal Rahim, Aftab Ahmad Khan, Muhammad Riaz: Novel Thiosemicarbazide-Oxadiazole Hybrids as the unprecedented inhibitors of yeast α -glucosidase and In Silico Binding Analysis. *RSC Advances.* 2016, 6, 33733-33742.
79. Uzma Salar, Muhammad Taha, Nor Hadiani Ismail, Khalid Mohammed Khan, Syahrul Imran, Shahnaz Perveen, **Abdul Wadood**, Muhammad Riaz: Thiadiazole derivatives as New Class of β -Glucuronidase Inhibitors. *Bioorg. Med. Chem.* 2016, 1909-1918.
80. Asad Ali, Anis Ur Rehman, Muhammad Ateeq, Farhat Ullah, Uzma Rasheed Mughal and **Abdul Wadood**. Conventional versus microwave assisted synthesis, molecular docking studies and in vitro evaluation of benzohydrazide derivatives as new acetylcholinesterase and butyrylcholinesterase inhibitors. *Med. Chem.* 2016, 6, 9.
81. Yahia Nasser Mabkhot, Fatima Alatibi, Nahed Nasser E El-Sayed, Salim Al-Showiman, Nabila Abdelshafy Kheder, **Abdul Wadood**, Abdur Rauf, Saud Bawazeer, Taibi Ben Hadda:

Antimicrobial Activity of Some Novel Armed Thiophene Derivatives and Petra/Osiris/Molinspiration (POM) Analyses. *Molecules*. 2016, 21, 222.

82. Muhammad Taha, Nor Hadiani Ismail, Syahrul Imran, Muhammad Helmi Mohamad, **Abdul Wadood**, Fazal Rahim, Syed Muhammad Saad, Ashfaq ur Rehman, Khalid Mohammed Khan: Synthesis, α -Glucosidase inhibitory, Cytotoxicity and Docking Studies of 2-Aryl-7-methylbenzimidazoles. *Bioorg. Chem.* 2016, 65, 100-109.
83. Reaz Uddin, Syed Sikander Azam, **Abdul Wadood**, Waqasuddin Khan, Umar Farooq, Ajmal Khan: Computational identification of potential drug targets against Mycobacterium leprae. *Med. Chem. Res.* 2016, 25, 473-481.
84. Assem Barakat, Hazem A. Ghabbour, Abdullah Mohammed Al-Majid, Qurat-ul-ain, Rehan Imad, KulsoomJavaid, Nimra Naveed Shaikh, Sammer Yousuf, M. Iqbal Choudhary, **Abdul Wadood**: Synthesis, X-Ray Crystal Structures, Biological Evaluation, and Molecular Docking Studies of a Series of Barbiturate Derivatives. *J. Chem. (Hindawi Publisher)*. 2016. Article ID 8517243.
85. Eunji Lee, Obaid Ur Rahman, Muhammad Tariq Masood Khan, **Abdul Wadood**, Muhammad Naeem, Changsoo Kang, Musharraf Jelani: Whole exome analysis reveals a novel missense PNPLA1 variant that causes autosomal recessive congenital ichthyosis in a Pakistani family. *J. Dermatol. Sci.* 2016, 82, 46-48.
86. Ajmal Khan, Jamshed Hashim, Nuzhat Arshad, Ijaz Khan, Naureen Siddiqui, **Abdul Wadood**, Muzaffar Ali, Fiza Arshad, Khalid Mohammed Khan, Muhammad I Choudhary: Dihydropyrimidine Based Hydrazine Dihydrochloride Derivatives as Potent Urease *Inhibitors*. *Bioorg. Chem.* 2016, 64, 85-96.
87. Nik Khairunissa Nik Abdullah Zawawi, M. Taha, NorizanAhmat, **Abdul Wadood**, Nor Hadiani Ismail, Fazal Rahim, Syed Sikander Azam, Noraishah Abdullah: Benzimidazole Derivatives as New α -Glucosidase Inhibitors and In Silico Studies. *Bioorg. Chem.* 2016, 64, 29-36.

2015

88. Muhammad Taha, Nor Hadiani Ismail, Syahrul Imran, **Abdul Wadood**, Fazal Rahim, Muhammad Riaz: Synthesis of Potent Urease Inhibitors Based on Disulphide Scaffold and Their Molecular Docking Studies. *Bioor. Med. Chem.* 2015, 23, 7211-7218.
89. Assem Barakat, Saied M. Soliman, Abdullah Mohammed Al-Majid, GehadLotfy, Hazem A. Ghabbour, Hoong-Kun Fun, Sammer Yousuf, M. Iqbal Choudhary, **Abdul Wadood**: Synthesis

and structure investigation of novel pyrimidine-2,4,6-trione derivatives of highly potential biological activity as anti-diabetic agent. *J. Mol. Struct.* 2015, 1098, 365-376.

90. Assem Barakat, Abdullah Mohammed Al-Majid, Saied M Soliman, GehadLotfy, Hazem A. Ghabbour, Hoong-Kun Fun, **Abdul Wadood**, Joseph C Sloop, Ismail Warad: *New Diethyl Ammonium Salt of Thiobarbituric Acid Derivative: Synthesis, Molecular Structure Investigations and Docking Studies.* *Molecules.* 2015, 20, 20642-20658.
91. Fazal Rahim, Khalid Zaman, Hayat Ullah, Muhammad Taha, **Abdul Wadood**, Muhammad Tariq Javed, Wajid Rehman, Muhammad Ashraf, Reaz Uddin, Imad uddin, Humna Asghar, Aftab Ahmad Khan, Khalid M. Khan: *Synthesis of 4-Thiazolidinone Analogs as Potent in Vitro Anti-urease Agents.* *Bioorg. Chem.* 2015, 63, 123-131.
92. Nik Khairunissa Nik Abdullah Zawawi, M. Taha, NorizanAhmat, Nor Hadiani Ismail, **Abdul Wadood**, F. Rahim, A. Ur Rehman: *Synthesis, in vitro evaluation and molecular docking studies of biscoumarin thiourea as a new inhibitor of α -Glucosidases.* *Bioorg. Chem.* 2015, 63, 36-44.
93. Nik Khairunissa, Nik AbdullliahZawawi, Muhammad Taha, NorizanAhmat, **Abdul Wadood**, Nor Hadiani Ismail, Fazal Rahim, Muhammad Ali, Norishah Abdullah, Khalid Muhammad Khan. *Novel 2,5-disubstituted-1,3,4-oxadiazoles with benzimidazole backbone: A new class of β -glucuronidase inhibitors and in silico studies.* *Bioorg. Med. Chem.* 2015, 23, 3119-3125.
94. Zaheer Ul-Haq, Sana Gul, SamanUsmani, **Abdul Wadood**, Waqasuddin Khan: *Binding Site Identification and Role of Permanent Water Molecule of PIM-3 Kinase: A Molecular Dynamics Study.* *J. Mol. Graph. Model.* 2015, 62, 276-282.
95. Muhammad Taha, Nor Hadiani Ismail, KulsoomJavaid, Syahrul Imran, El HassaneAnouar, **Abdul wadood**, Atia-tul-Wahab, Muhammad Ali, K. M. Khan, Syed Muhammad Saad, Fazal Rahim, M Iqbal Choudhary: *Evaluation of 2-Indolcarbohydrazones as Potent α -Glucosidase inhibitors, In Silico Studies and DFT based Stereochemical Predictions.* *Bioorg. Chem.* 2015, 63, 24-35.
96. Assem Barakat, Mohammad Shahidul Islam, Abdullah Mohammed Al-Majid, Hazem A. Ghabbour, Hoong-Kun Fun, KulsoomJaved, Rehan Imad, Sammer Yousuf, M Iqbal Choudhary, **Abdul Wadood**: *Synthesis, In vitro Biological Activities and In Silico Study of Dihydropyrimidines Derivatives.* *Bioorg. Med. Chem.* 2015, 23, 6740-6748.
97. Muhammad Taha, Nor Hadiani Ismail, Syahrul Imran, **Abdul Wadood**, Fazal Rahim, Muhammad Ali, Ashfaq Ur Rehman: *Novel Quinoline Derivatives as Potent In Vitro α -*

- Glucosidase Inhibitors: In Silico Studies and SAR Predictions. *Med. Chem. Commun.* 2015, 6, 1826-1836.
98. Fazal Rahim, Khadim Ullah, Hayat Ullah, **Abdul Wadood**, Muhammad Taha, Ashfaq Ur Rehman, Imad Uddin, Muhammad Ashraf, Ayesha Shaukat, Wajid Rehman, Shafqat Hussain, Khalid Mohammed Khan: Triazinoindoleanalogs as potent inhibitors of α -glucosidase: Synthesis, biological evaluation and molecular docking studies. *Bioorg. Chem.* 2015, 58, 81-87.
99. Fazal Rahim, Hayat Ullah, Muhammad Tariq Javid, **Abdul Wadood**, Muhammad Taha, Muhammad Ashraf, Ayesha Shaukat, Muhammad Junaid, Shafqat Hussain, Wajid Rehman, Rashad Mehmood, Muhammad Sajid, Muhammad Naseem Khan, Khalid Mohammed Khan: *Synthesis, in vitro evaluation and molecular docking studies of thiazole derivatives as new inhibitors of α -glucosidase.* *Bioorg. Chem.* 2015, 62, 15-21.
100. Fazal Rahim, Muhammad Tariq Javid, Hayat Ullah, **Abdul Wadood**, M. Taha, Muhammad Ashraf, Qurat-ul-Ain, Muhammad Anas Khan, Fahad Khan, Salma Mirza, Khalid M. Khan. Synthesis molecular docking, acetylcholinesterase and butyrylcholinesterase inhibitory potential of thiazoleanalogs as new inhibitors for Alzheimer disease. *Bioorg. Chem.* 2015, 62, 106-116.
101. Naveed Muhammad, Ram Lal Shrestha, A. Adhikari, **Abdul Wadood**, Haroon Khan, Amir Zada Khan, F.Maione, N.Mascolo, V. De Feo: First evidence of the analgesic activity of govaniadine, an alkaloid isolated from *Corydalis govaniensis* Wall. *Nat. Prod. Res.* 2015, 29, 430-437.
102. Assem Barakat, Abdullah Mohammed Al-Majid, Saied M Soliman, Yahia Nasser Mabkhot, M Ali, Hazem A Ghabbour, Hoong-Kun Fun, **Abdul Wadood**: Structural and spectral investigations of the recently synthesized chalcone (E)-3-mesityl-1-(naphthalen-2-yl) prop-2-en-1-one, a potential chemotherapeutic agent. *Chem. Central J.* 2015, 9, 35.
103. Umer Rashid, Syed Fahad Hassan, Samina Nazir, **Abdul Wadood**, Muhammad Waseem, Farzana Latif Ansari: Synthesis, docking studies, and in silico ADMET predictions of some new derivatives of pyrimidine as potential KSP inhibitors. *Med. Chem. Res.* 2015, 24, 304-315.
104. Reaz Uddin, Kiran Saeed, Waqasuddin Khan, Syed Sikander Azam, **Abdul Wadood**: Metabolic pathway analysis approach: Identification of novel therapeutic target against methicillin resistant *Staphylococcus aureus*. *Gene*, 2015, 213-226.

105. Fazal Rahim, Fazal Malik, Hayat Ullah, **Abdul Wadood**, Fahad Khan, Muhammad Tariq Javid, Muhammad Taha, Wajid Rehman, Ashfaq Ur Rehman, Khalid Muhammad Khan. Isatin based Schiff bases as inhibitors of α -glucosidase: Synthesis, characterization, in vitro evaluation and molecular docking studies. *Bioorg. Chem.* 2015, 60, 42-48.
106. Ashfaq Ur Rehman, T. K. Muhammad, **Abdul Wadood**, K. Qaiser, Zahid Ullah, A. Ayaz, B. J. Syed, M. Naeem, B. S. Syed, J. M. A. Bilal, R. Hamid: Exploring the binding pattern of predicted potent inhibitor to sirR_mtb; Modeling and structure-base virtual screening of sirR protein of Mycobacterium Tuberculosis (MTB). *Int. J. Comput. Bioinf. In Silico Model.* 2015, 4, 651-658.

2014

107. **Abdul Wadood**, Muhammad Riaz, Reaz Uddin, Zaheer Ul-Haq: In Silico 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. *PLOS ONE*, 2014, 9, e89109.
108. **Abdul Wadood**, Syed Babar Jamal, Muhammad Riaz, Asif Mir: *Computational analysis of benzofuran-2-carboxylic acids as potent Pim-1 kinase inhibitors*. *Pharm. Biol.* 2014, 52, 1170-1178.
109. **Abdul Wadood**, Lubna Shah, Muhammad Riaz, Ashfaq Ur Rehman, Nasir Ahmad, Amir Fahira, Muhammad Naeem, Momin Khan, Sahib Gul. Exploring binding modes of 5-substituted 1h-Tetrazoles as cyclooxygenase inhibitors: A Molecular docking study. *J. Appl. Environ. Biol. Sci.* 2014, 4, 113-122.
110. **Abdul Wadood**, Huma, Zahid Ullah, Muhammad Riaz, Sulaiman Shams, MehreenGufuran, Amir Fahira, Muhammad Naeem, Sahib Gul, Ayaz Ahmad. Structural Modeling and Molecular Dynamics Simulation Studies of Camel Milk Kappa Casein Protein. *Int. J. Comput. Bioinf. In Silico Model.* 2014, 3, 483-490.
111. **Abdul Wadood**, Ashfaq Ur Rehman, Sulaiman Shams, Momin Khan, Taj Ur Rahman, Syed Babar Jamal, Asifullah Khan, Ayaz Ahmad, Farman Ali: *Homology Modeling, Molecular Dynamic Simulation and Phylogenetic Analysis of Human Transient Receptor Potential Melastatin 1 (TRPM1)*. *Int. J. Comput. Bioinf. In Silico Model.* 2014, 3, 381-387.
112. Abdur Rauf, Ghias Uddin, Bina S. Siddiqui, Ajmal Khan, Haroon Khan, Mohammad Arfan, Naveed Muhammad, **Abdul Wadood**. In-vivo antinociceptive, anti-inflammatory and

- antipyretic activity of pistagremic acid isolated from Pistaciaintegerrima. *Phytomedicine*, 2014, 21, 1509-1515.
113. Muhammad Junaid, Ziyad Tariq Muhseen, Ata Ullah, **Abdul Wadood**, Junjun Liu, Houjin Zhang: Molecular modeling and molecular dynamics simulation study of the human Rab9 and RhoBTB3 C-terminus complex. *Bioinformation*. 2014, 10, 753-759.
114. Bilal J M Alrawi, Ashfaq Ur Rehman, Ayaz Ahmad, Asma Mohammed, Syed Babar Jamal, Nasir Ahmad, **Abdul Wadood**, Lubna Shah: Prediction of Binding Mode of Bisphenol-A (A Carcinogen) in Estrogen and Testosterone Receptors by Applying Computational Docking Approach. *J. Appl. Environ. Biol. Sci.* 2014, 4, 101-105.
115. Riaz Ahmad Khan, Ashfaq Ur Rahman, Ayaz Ahmad, Muhammad Jaseem, Abdul Jabbar, Shad Ali Khan, Amjad Iqbal, Nasir Ahmad, **Abdul Wadood**, Taj Ur Rahman: Prevalence and Antibiotic Susceptibility Profile of Methicillin-Resistant Staphylococcus aureus (MRSA) Isolated from Different Clinical Samples in District Peshawar. *J. Appl. Environ. Biol. Sci.* 2014, 4, 40-46.
116. Naveed Muhammad, Muhammad Saeed, Ajmal Khan, Achyut Adhikari, **Abdul Wadood**, Khalid Mohammed Khan, Vincenzo De Feo: A New Urease Inhibitor from Viola betonicifolia. *Molecules*, 2014, 19, 16770-16778.
117. Sajid Ali, Ayaz Ahmad, Raham Sher Khan, Sanaullah Khan, Muhammad Hamayun, Sumera Afzal Khan, Amjad Iqbal, Abid Ali Khan, **Abdul Wadood**, Taj Ur Rahman, Ali HydarBaig: *Genotyping of HCV RNA Reveals That 3a Is the Most Prevalent Genotype in Mardan, Pakistan*. *Advances in Virology*, 2014, DOI:10.1155/2014/606201
118. Khalid Mohammed Khan, Fazal Rahim, **Abdul Wadood**, Muhammad Taha, Momin Khan, ShaguftaNaureen, Nida Ambreen, Shafqat Hussain, Shahnaz Perveen, Mohammad Iqbal Choudhary: *Evaluation of bisindole as potent β -glucuronidase inhibitors: Synthesis and in silico based studies*. *Bioorg. Med. Chem. Lett.* 2014, 24, 1825-1829.
119. Muhammad Bilal, Ayaz Ahmad, Khalid Khan, Nasir Ahmad, Ashfaq Ur Rehman, Muhammad Junaid, Amjad Iqbal, Waheed Ahmad, **Abdul Wadood**, Taj Ur Rehman: Computational Prediction Of Micro-RNAs In Hepatitis B Virus Genome. *J. Appl. Environ. Biol. Sci.* 2014, 4, 106-113.
120. Momin Khan, Muhammad Yousaf, **Abdul Wadood**, Muhammad Junaid, Muhammad Ashraf, Umer Alam, Muhammad Ali, Muhammad Arshad, Zahid Hussain, Khalid Mohammed

- Khan: Discovery of novel oxindole derivatives as potent α -glucosidase inhibitors. *Bioorg. Med. Chem.* 2014, 22, 3441-3448.
121. Khalid Mohammed Khan, Fazal Rahim, **Abdul Wadood**, Naveen Kosar, Muhammad Taha, Salima Lalani, Aisha Khan, Muhammad Imran Fakhri, Muhammad Junaid, Wajid Rehman, Momin Khan, Shahnaz Perveen, Muhammad Sajid, M Iqbal Choudhary: Synthesis and molecular docking studies of potent α -glucosidase inhibitors based on biscoumarin skeleton. *Eur. J. Med. Chem.* 2014, 81, 245-252.
122. **Abdul Wadood**, Muhammad Riaz, Syed Babar Jamal, Masaud Shah: *Interactions of ketoamide inhibitors on HCV NS3/4A protease target: Molecular docking studies.* *Mol. Biol. Rep.* 2014, 41, 337-345.
123. **Abdul Wadood**, Muhammad Riaz, Amir Ul Mulk, Momin Khan, Sobia Ahsan Haleem, Sulaiman Shams, Sahib Gul, Ayaz Ahmed, Muhammad Qasim, Farman Ali, Zaheer Ul-Haq: *Design of New and Potent Diethyl Thiobarbiturates as Urease Inhibitors: A Computational Approach.* *Bioinformation*, 2014, 10, 299-307.
124. Saleha Suleman Khan, Ajmal Khan, Afsar Khan, **Abdul Wadood**, Umar Farooq, Amir Ahmed, Aqib Zahoor, Viqar Uddin Ahmad, Bilge Sener, NurgunErdemoglu: *Urease inhibitory activity of ursane type sulfated saponins from the aerial parts of Zygophyllumfabago Linn.* *Phytomedicine*, 2014, 21, 379-382.
125. Taj Ur Rahman, G. Uddin, K. F. Khattak, W. Liaqat, G. Mohammad, M. I. Choudhary, **Abdul Wadood**, Ayaz Ahmad. Isolation and characterization of a novel ester from seed of *Indigoferaheterantha* (Wall). *J. Nat. Prod.* (ISSN 0974-5211) 2014, 7, 104-112.
126. Taj Ur Rahman, GhiasUddin, Wajiha Liaqat, M. Iqbal Choudhary, **Abdul Wadood**, Ghulam Mohammad, Ayaz Ahmed: Pharmacological investigations of *Eclipta alba* extract fractions (Whole Plant). *Indo Amrican J. Pharm. Res.* 2014, 4. (ISSN NO 2231-6876)
127. Sulaiman Shams, Abdur-Rahman, Abdul Haq, Hammad Hassan, Sahib Gul Afridi, **Abdul Wadood**. Prevalence of Tuberculosis in District KharBajaur Agency, Khyber Pakhtunkhwa Pakistan. *Biochem. Anal. Biochem.* 2014, 3, 1.

2013

128. Masaud Shah, **Abdul Wadood**, Ziaur Rahman, Tayyab Husnain: *Interaction and Inhibition of Dengue Envelope Glycoprotein with Mammalian Receptor DC-Sign, an In-Silico Approach.* *PLoS ONE*, 2013; 8, e59211.

129. **Abdul Wadood**, Zaheer- Ulhaq: *In silico identification of novel inhibitors against Plasmodium falciparum dihydroorotate dehydrogenase*. J. Mol. Graph. Model. 2013, 40, 40-47.
130. **Abdul Wadood**, N Ahmed, L Shah, A Ahmad, H Hassan, S Shams: *In-silico drug design: An approach which revolutionarised the drug discovery process*. OA Drug Des. Deliv. 2013, 1, 3.
131. **Abdul Wadood**, Shandana Ali, Muhammad Riaz, Syed Babar Jamal, Taj Ur Rehman, Sahib Gul, Mukhtiar Hassan: *Molecular Docking Study of 5-substituted-8-methyl-2H-pyrido [1, 2-a] pyrimidine-2, 4 (3H) – diones As Inhibitors of Basilluspasteurii urease*. Pakhtunkhwa J. Life Sci. 2013, 1, 145-153.
132. **Abdul Wadood**, Nasir Ahmad, Muhammad Riaz, Sulaiman Shams, JavedAnwer, Ayaz Ahmad: *Homology Modeling and Molecular Dynamics study of Candida Albicans Heat Shock Protein 21, a Potential Target Protein for Antifungal Drug Development*. Int. J. Sci. 2013, 2.
133. **Abdul Wadood**, MehreenGhufran, Syed Babar Jamal, Muhammad Naeem, Ajmal Khan, Rukhsana Ghaffar, Asnad: *Asnad. Phytochemical Analysis of Medicinal Plants Occurring in Local Area of Mardan*. Biochem. Anal. Biochem. 2013, 2.
134. Gowhar Ali, Fazal Subhan, **Abdul Wadood**, Ajmal khan, Nasir Ullah, Nazar Ul Islam and 2Ikhtiar Khan: *Pharmacological evaluation, molecular docking and dynamics simulation studies of salicyl alcohol nitrogen containing derivatives*. African J. Pharm. Pharmacol. 2013, 7, 585-596.
135. Sobia Ahsan Halim, Omer Mohamed Abdalla, M Ahmed Mesaik, **Abdul Wadood**, Zaheer Ul-Haq, Maria Kontoyianni: *Identification of novel Interleukin-2 inhibitors through computational approaches*. Mol. Div. 2013, 17, 345-355.
136. **Abdul Wadood**, Muhammad Riaz, Syed Babar Jamal, Masaud Shah, Muhammad Arif Lodhi: *Molecular docking study of P4-Benzoxaborolesubstituted ligands as inhibitors of HCV NS3/4A protease*. Bioinformation, 2013, 9, 309-314.
137. Umer Rashid, Iram Batool, **Abdul Wadood**, Ajmal Khan, Zaheer-ul-Haq, Muhammad Iqbal Chaudhary, Farzana Latif Ansari: *Structure based virtual screening-driven identification of monastrol as a potent urease inhibitor*. J. Mol. Graph. Mod. 2013, 43, 47-57.
138. Muhammad Arif Lodhi, Zaheer Ul-Haq, **Abdul Wadood**, Sajjed Iqbal, Khalid Muhammad Khan, Atta-Ur-Rahman, Muhammad Iqbal Choudhary: *Erratum to: Three-*

dimensional quantitative structure–activity relationship (CoMSIA) analysis of bis-coumerine analogues as urease inhibitors. Med. Chem. Res. 2013, 22, 498-504.

2012

139. **Abdul Wadood**, Syed Abid Ali, Rabia Sattar, Muhammad Arif Lodhi, Zaheer Ul-Haq: *A Novel Pharmacophore Model to Identify Leads for Simultaneous Inhibition of Anti-coagulation and Anti-inflammatory Activities of Snake Venom Phospholipase A2.* Chem. Biol. Drug Des. 2012, 79, 431-441.
140. Syed Sikander Azam, Reaz Uddin, **Abdul Wadood**. *Structure and dynamics of alpha-glucosidase through molecular dynamics simulation studies.* J. Mol. Liquid. 2012, 174, 58-62.

2011

141. Zaheer Ul Haq, Reaz Uddin, Lam Kok Wai, **Abdul Wadood**, Nordin Haji Lajis: *Docking and 3D-QSAR modeling of cyclin-dependent kinase 5/p25 inhibitors.* J. Mol. Model. 2011, 17, 1149, 1161.
142. Khalid Mohammed Khan, Muhammad Ali, **Abdul Wadood**, Zaheer-ul-Haq, Momin Khan, Muhammad Arif Lodhi, Shahnaz Perveen, Muhammad Iqbal Choudhary, Wolfgang Voelter: *Molecular modeling-based antioxidant arylidene barbiturates as urease inhibitors.* J. Mol. Graph. Model. 2011, 30, 153-156.

2010

143. 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, 45, 5200-5207.
144. Obaid-ur-Rahman Abid, Tariq Mahmood Babar, FarukhIftakhar Ali, Shahzad Ahmed, **Abdul Wadood**, Nasim Hasan Rama, Reaz Uddin, Ajmal Khan, M. Iqbal Choudhary: *Identification of Novel Urease Inhibitors by High-Throughput Virtual and in Vitro Screening.* ACS Med. Chem. Lett. 2010, 1, 145-149.
145. Khalid M Khan, **Abdul Wadood**, Muhammad Ali, Zia-Ullah, Zaheer Ul-Haq, M Arif Lodhi, Momin Khan, Shahnaz Perveen, M Iqbal Choudhary: *Identification of potent urease inhibitors via*

ligand- and structure-based virtual screening and in vitro assays. J. Mol. Graph. Model. 2010, 28, 792-798.

2009

146. Z Ul-Haq, **Abdul Wadood**: *Prediction of Binding Affinities for Hydroxamic Acid Derivatives as Urease Inhibitors by Molecular Docking and 3D-QSAR Studies*. Lett. Drug Des. Discov. 2009, 6, 93-100.
147. Zaheer- Ul-Haq, **Abdul Wadood**, Reaz Uddin: *CoMFA and CoMSIA 3D-QSAR analysis on hydroxamic acid derivatives as urease inhibitors*. J. Enz. Inhib. Med. Chem. 2009, 24, 272-278.
148. Farzana Latif Ansari, **Abdul Wadood**, Ahsan Ullah, Fatima Iftikhar, Zaheer Ul-Haq: *In silico studies of urease inhibitors to explore ligand-enzyme interactions*. J. Enz. Inhib. Med. Chem. 2009, 24, 151-156.

Workshops/Conferences

- 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. Panjwani 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.
- 22-25th Aug. 2016 Oral presentation in 27th National and 15th International Chemistry Conference University of Malakand.
- 15-18th Dec. 2016 Participation in 14th Euroasia Conferece on Chemical Sciences Malakand University, Pakistan.
- 27-29 Sep. 2017 Oral presentation in three days national conference on Computational Biology and Genomics, Hazara University Mansehra, Pakistan.

References

1. Prof. Dr.Raham Sher

Department of Biotechnology, Abdul Wali Khan University Mardan, Mardan, Pakistan.

hamayun@awkum.edu.pk

2. Prof. Dr. Khalid M Khan

HEJ Research Institute of Chemistry, University of Karachi, Pakistan.

khalid.khan@iccs.edu

3. Assoc. Prof. Dr. Zaheer ul-Haq

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

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