

1) **List of Research Publications (Total Impact Factor 65.777)**

List of Publications				
	No.		Impact Factor	Published In
Submitted	(1)	Zaheer-ul-Haq, Sobia Ahsan Halim and Reaz Uddin, Benchmarking Docking and Scoring Protocol for the Identification of Potential Acetylcholinesterase Inhibitors, <i>J. Mol. Graph. Model</i>		USA
	(2)	Rama, N. H., Wadood, A., Abid, O., Babar, T. M., Ali, F. I., Ahmed, S., Zaheer-ul-Haq , Reaz-uddin, Khan, A., and Choudhary, M. I., Identification of novel urease inhibitors by high-throughput virtual screening, <i>J. Med. Chem.</i>		USA
	(3)	Khan, K. M., Zia-Ullah, Ali, M., Wadood, A., Zaheer-ul-Haq , Lodhi, M. A., Perveen, S., Choudhary, M. I. and Atta-ur-Rahman, Identification of potent urease inhibitors via ligand- and structure-based virtual screening and in vitro assays, <i>J. Mol. Graph. Model.</i> ,		USA
2009	(4)	Mesaik, M. A. , Zaheer-ul-Haq, Choudhary M. I, Shahnaz S., Murad and Ahmad A. Immunosuppressive Activity of Buxidin and E-Buxenone from <i>Buxus hyrcana</i> , <i>Chem. Biol. Drug Design.</i> (In Press)	2.38	England
	(5)	Zaheer-ul-Haq, Shamshad Zarina, Waqasuddin Khan , Rabia Sattar and Syed Tarique Moin., Template-Based Structure Prediction and Molecular Dynamics Simulation Study of Two Mammalian Aspartyl-tRNA Synthetases, <i>J. Mol. Graph. Model.</i> (In Press)	2.34	USA
	(6)	Zaheer-ul-Haq , Uzma Mahmood and Bushra Jahangir, Ligand-based 3D-QSAR Studies of Physostigmine Analogues as Acetylcholinesterase Inhibitors, <i>Chem. Biol. Drug Design.</i> , (In Press)	2.38	England
	(7)	Zaheer-ul-Haq , Hadi H., Moin T. and Choudhary, M. I., Molecular Dynamics Simulation of Human Acetylcholinesterase Complex with its Potent Natural Inhibitor, <i>J. Enz. Inhib. Med. Chem.</i> (In Press)	1.343	England
	(8)	Zaheer-ul-Haq and Wadood A., Prediction of Binding Affinities for Hydroxamic Acid Derivatives	0.50	Netherlands

		as Urease Inhibitors by Molecular Docking and 3D-QSAR Studies, <i>Lett. Drug Des. Discov.</i> 6, 93-100.		
	(9)	Ansari F. L., Wadood A., Ullah A., Iftikhar F. and Zaheer-ul-Haq , <i>In Silico</i> Studies of Urease Inhibitors to Explore Ligand-Enzyme Interactions. <i>J. Enz. Inhib. Med. Chem.</i> , 24, 151-156.	1.343	England
	(10)	Zaheer-ul-Haq and Iqbal S., Receptor-Based 3D-QSAR Study for Recognizing True Binding Mode of Mercaptoacyldipeptides at The Active Site of Neutral Endopeptidase, <i>Med. Chem.</i> , 5, 50-65.	NA	Netherlands
	(11)	Zaheer-ul-Haq , Wadood A. and Uddin R., CoMFA and CoMSIA 3D-QSAR Analysis on Hydroxamic Acid Derivatives as Urease Inhibitors, <i>J. Enz. Inhib. Med. Chem.</i> , 24, 272-278.	1.343	England
2008	(12)	Zaheer-ul-Haq , Uddin R., Yuan H. and Madura J. D. Receptor-Based Modeling and 3D-QSAR for a Quantitative Production of the Butyrylcholinesterase Inhibitors Based on Genetic Algorithm, <i>J. Chem. Inf. Mod.</i> , 48, 1092-03.	3.643	USA
	(13)	Zaheer-ul-Haq , Lodhi, M. A., Nawaz, S. A., Iqbal, S., Khan, K. M., Rode, B. M., Atta-ur-Rahman and Choudhary, M. I., 3D-QSAR CoMFA Studies on Bis-coumarine Analogues As Urease Inhibitors: A Strategic Design In Anti-urease Agents. <i>Bioorg. Med. Chem.</i> 16, 3456-3461.	2.662	England
2007	(14)	Zaheer-ul-Haq , Dalal, P., Aronson. N. N., Madura, J. D., Family 18 Chitolectins: Comparison of MGP40 and HUMGP39, <i>Biochem. Biophys. Res. Commun.</i> , 359, 2, 221-226.	2.855	USA
	(15)	Choudhary A. M. A., Akhtar N., Zaheer-ul-Haq, Haleem, M. A. Computer Aided Drug Design of NF-033 for Aids Treatment, <i>Int. J. Biol. Biotech.</i> 4, 335-346.		Pakistan
2006	(16)	Mesaik M. A., Zaheer-ul-Haq , Choudhary M. I., Murad S., Ismail Z., Abdullah N. R., Atta-ur-Rahman and Ahmad A. Biological and Molecular Docking Studies on Coagulin-H: IL-2 Natural Inhibitor, <i>Molecular Immunology</i> , 43, 1855-63.	4.768	England

	(17)	Khan K. M., Ullah, Z., Lodhi, M. A., Ali M., Choudhary, M. I., Atta-ur-Rahman, and Zaheer-ul-Haq , Successful Computer Guided Planned Synthesis of (4R)-thiazolidine Carboxylic Acid and its 2-Substituted Analogues as Urease Inhibitors, <i>Molecular Diversity</i> , 10, 223-231.	2.534	Netherlands
2005	(18)	Choudhary, M. I., Nawaz, S. A., Zaheer-ul-Haq , Saima J., Atta-ur-Rahman, M. N. Ghayur, Anwar-ul-Hassan Gilani, Viqar Uddin Ahmad and A. Ahmed, Juliflorine: A Novel, Natural and Peripheral Anionic-site Binding Inhibitor of Acetylcholinesterase with Calcium- channel Blocking Potential, A Lead for Alzheimer's Disease Therapy, <i>Biochem. Biophys. Res. Commun.</i> , 332, 1171-1179.	2.855	USA
	(19)	Gilani, A. H., Ghayur, M. N., Khalid, A., Zaheer-ul-Haq , Choudhary, M. I. and Atta-ur-Rahman, Presence of Antispasmodic, Antidiarrhoeal, Antisecretory, and Acetylcholinesterase, Inhibitory Constituents in <i>Sarcococca saligna</i> , <i>Planta Med.</i> , 71, 120-125.	1.746	Germany
	(20)	Choudhary, M. I., Nawaz, S. A., Zaheer-ul-Haq , Lodhi, M. A., Ghayur, M. N., Jalil, S., Riaz, N., Yousuf, S., Malik, A., Gilani, A. H., Atta-ur-Rahman, Withanolides, a new class of natural cholinesterase inhibitors with calcium antagonistic properties, <i>Biochem. Biophys. Res. Commun.</i> , 334, 267-287.	2.855	USA
2004	(21)	Khalid, A., Zaheer-ul-Haq , Anjum S., Khan, M. R., Atta-ur-Rahman and Choudhary, M. I., Kinetics and Structure-Activity Relationship studies on Steroidal Alkaloids That Inhibit Cholinesterases, <i>Bioorg. Med. Chem.</i> 12(9), 1995-2003.	2.624	England
	(22)	Atta-ur-Rahman, Zaheer-ul-Haq , Feroz, F., Khalid, A., Nawaz, S. A., Khan, M. R. and Choudhary, M. I., New Cholinesterase Inhibiting Steroidal Alkaloids from <i>Sarcococca saligna</i> , <i>Helv. Chim. Acta</i> , 87, 439-48.	1.861	Switzerland

	(23)	Atta-ur-Rahman, Feroz, F., Naeem, I., Zaheer-ul-Haq , Nawaz, S. A., Khan, N., Khan, M. R. and Choudhary, M. I., New Pregnane-Type Steroidal Alkaloids from <i>Sarcococca saligna</i> and their cholinesterase Inhibitory Activity, <i>Steroids</i> 69, 735–741.	2.849	USA
	(24)	Khalid, A., Zaheer-ul-Haq , Ghayur, M. N., Feroz, F., Atta-ur-Rahman, Gilani, A. H. and Choudhary, M. I., Cholinesterase Inhibitory and Spasmolytic Potential of Steroidal Alkaloids, <i>J. Steroid Biochem. & Mol. Bio.</i> 92, 477-484.	2.825	England
	(25)	Anjum S., Atta-ur-Rahman, Choudhary M. I., Khalid A., Zaheer-ul-Haq , Feroz F. Interesting SAR studies of pregnane alkaloids isolated from genus <i>Sarcococca</i> against cholinesterase enzymes, <i>Iranian Journal of Pharmaceutical Research</i> , 2:16.		Iran
2003	(26)	Zaheer-ul-Haq , Wellenzohn, B., Liedl, K. R., and Rode, B. M., Molecular Docking Studies of Natural Cholinesterase-Inhibiting Steroidal Alkaloids from <i>Sarcococca saligna</i> . <i>J. Med. Chem.</i> 46(23):5087-90.	4.895	USA
	(27)	Zaheer-ul-Haq , Wellenzohn, B., Tonmunpheap, S., Khalid, A., Choudhary, M. I. and Rode, B. M., 3D-QSAR Studies on Natural Acetyl-cholinesterase Inhibitors of <i>Sarcococca saligna</i> by Comparative Molecular Field Analysis (CoMFA). <i>Bioorg. Med. Chem. Lett.</i> , 13, 4375–4380.	2.604	England
	(28)	Ghayur, M. N., Gilani, A. H., Khalid. A., Choudhary, M. I., Zaheer-ul-Haq , Kalauni, S. K., Atta-ur-Rahman, The Presence of Calcium Channel Blocking and Acetylcholinesterase Inhibitory Constituents in <i>Sarcococca Saligna</i> . <i>FASEB J.</i> , 17: A238.	13.02	USA
	(29)	Atta-ur-Rahman, Feroz, F., Zaheer-ul-Haq , Nawaz, S. A., Khan, M. R. and Choudhary, M. I., New Steroidal Alkaloids From <i>Sarcococca saligna</i> , <i>Nat Prod Res.</i> 17(4): 235.	0.798	England
2002	(30)	Atta-ur-Rahman, Zaheer-ul-Haq , Khalid, A. Anjum, S. Khan, M. R. and Choudhary M. I., Pregnane-type Steroidal Alkaloids of <i>Sarcococca saligna</i> : A New class of Cholinesterases Inhibitors. <i>Helv. Chim. Acta</i> , 85, 678-688.	1.861	Switzerland

In Preparation	(31)	Zaheer-ul-Haq, Uzma Mahmood and Rabia Sattar, Comparative Molecular Modeling Study of Butyrylcholinesterase, <i>Protein & Peptide Lett.</i>		
	(32)	Imtiaz Khan, Reaz Uddin, Sajid Ali, M. Iqbal Choudhary, Zaheer-ul-Haq and Nasim Hasan Rama, Synthesis, urease inhibition and antioxidant activities of Some 1,2,4-triazole and 1,3,4-thiadiazole derivatives, <i>Eur. J. Med. Chem.</i>		
	(33)	Khan, K. M., Nida Ambreen, Sobia Ahsan Halim, Zaheer-ul-Haq, Wadood, A., Khan, A., Naureen, S., Rasheed, S., Chaudhary, M. I. and Atta-ur-Rahman, Structure-Based Design, Synthesis and Biological Evaluation of Selective β -Glucuronidase Inhibitors.		
	(34)	Zaheer-ul-Haq, Moin, S. T., Khan, K. M. and Choudhary, M. I., Exploring Binding Patterns of Piperidines on Cholinesterase: A Molecular Dynamics Study,		
	(35)	Zaheer-ul-Haq and Sadaf Iqbal, Computational Insights into the Structural Features of XCE Enzyme Through Homology Modeling, MD Simulations, and Docking Studies: A Comparison With ECE-1		
	(36)	Asaad Khalid, Waqas Uddin, Zaheer-ul-Haq, Azim, M. K., Azizuddin, Atta-ur-Rahman and M. I. Choudhary, Experimental and Theoretical Investigations of Mechanism of Cholinesterases Inhibition by Natural Coumarins		
	(37)	Zaheer-ul-Haq, Waqasuddin Khan, Saima Kalsoom and Ansari, F. L., Exploratory Studies on the Interactions of Thiophene-2,3-dihydro-1,5-benzothiazepines-Cholinesterase Complexes by Docking and Molecular Dynamics Simulations, <i>Journal of Biomolecular Structure and Dynamics</i>		
	(38)	Atta-ur-Rahman, M. Nadeem Akhtar, Waqasuddin Khan, Zaheer-ul-Haq, M. I. Choudhary, Sarfraz A. Nawaz, Yoshisuke Tsuda and Bilge Sener, Bioassay-guided Isolation and Structural Insight of Butyrylcholinesterase Inhibitor from <i>Fritilaria imperialis</i> , <i>Chemistry and Biodiversity</i>		

B. Abstracts in Scientific Meetings:

(39) Reaz Uddin and Zaheer-ul-Haq, 3D-QSAR Study of Steroidal Alkaloid Analogues as Inhibitors of Butyrylcholinesterase, 233rd ACS National Meeting, held in Chicago, USA, on March 25-28, 2007.

(40) Sobia Ahsan Halim and Zaheer-ul-Haq, Modeling Aided Lead Design of Cytokine Inhibitors, 1st International Workshop-cum-Training Course on Molecular Medicine and Drug Research held in Dr. Panjwani Center For Molecular Medicine & Drug Research, University Of Karachi, on January 16 - 30, 2007.

(41) Abdul-Wadood & Zaheer-ul-Haq, Prediction of Binding Affinities for Hydroxamic Acid Derivatives as Urease Inhibitors by Molecular Docking and 3D-QSAR Studies, held in Dr. Panjwani Center For Molecular Medicine & Drug Research, University Of Karachi, on January 16 - 30, 2007.

(42) Afshan Naz, Naheed Akhter and Zaheer-ul-Haq, Comparative Molecular Docking Studies on Combretastatins A-4 Analogues of Microtubule Inhibitors, 1st International Workshop-cum-Training Course on Molecular Medicine and Drug Research held in Dr. Panjwani Center For Molecular Medicine & Drug Research, University Of Karachi, on January 16 - 30, 2007.

(43) Uzma Mahmood, Rabia Sattar and Zaheer-ul-Haq, held in Dr. Panjwani Center For Molecular Medicine & Drug Research, University Of Karachi, on January 16 - 30, 2007.

(44) Zaheer-ul-Haq, M. Arif Lodhi and M. Iqbal Choudhary, Insights into the Metal Chelating Mechanism in Biscoumerine Interaction Using Molecular Docking Simulation and Comparative Field Analysis, "20th "Darmstadt" Molecular Modeling Workshop" Computer-Chemie-Centrum, Erlangen, Germany, May 23 – 24, 2006.

(45) Zaheer-ul-Haq, and M. Iqbal Choudhary, The Role of Computational Chemistry in the Process of Drug Discovery, 6th International & 16th National Chemistry Conference, held in Bahauddin Zakariya University, Multan on April 6-8, 2006

(46) Sajjad Hussain, Nessar Ahmed, Zaheer-ul-Haq, M. Iqbal Chodhary and Mark Slevin, Identification and characterization of natural products as anti-angiogenic drug candidates. Manchester Metropolitan University, Research Institute for Health & Social Change (RIHSC) 2006 Annual Conference, Monday 3rd July 2006

(47) Zaheer-ul-Haq, Asaad Khalid and M. Iqbal Choudhary, Comparative Molecular Field Analysis (CoMFA) of Natural Cholinesterase-Inhibiting Steroidal Alkaloids, 2nd International Conference of the Division of Pharmaceutical and Drug Industry" held in Cairo, Egypt on March 6-10, 2005.

(48) Zaheer-ul-Haq, Khalid, A., Choudhary, M. I. and Atta-ur-Rahman, The Importance of Computational Chemistry in Drug Design: A CoMFA Approach to Steroidal Alkaloids Cholinesterase Inhibitors, 4th International & 14th National Chemistry Conference, The Chemical Society of Pakistan, May 16-18.

- (49) Gilani, A. H., Ghayur, M. N., Zaheer-ul-Haq, Atta-ur-Rahman, Cardiovascular tone Modulatory Action of *Sarcococca saligna*, Spring 2004 Meeting, Hulme Hall, University of Manchester, British Society for Cardiovascular Research.
- (50) Zaheer-ul-Haq, Wellenzohn, B., Tonmunphean, S., Khalid, A., Choudhary, M. I. and Rode, B. M. 3D-QSAR Studies on Natural Acetyl-cholinesterase Inhibitors of *Sarcococca saligna* by Comparative Molecular Field Analysis (CoMFA). 9th International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 10-13.
- (51) Khalid, Zaheer-ul-Haq, M. N. Ghayur, Atta-ur-Rahman, A. H. Gilani and M. I. Choudhary, Structural Basis of Acetylcholinesterase Inhibition by Steroidal Alkaloids, 9th International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 10-13.
- (52) F. Feroz, Atta-ur-Rahman, M.I. Choudhary, Zaheer-ul-Haq, S. A. Nawaz and M R. Khan, Structure Activity Relationship of Steroidal Alkaloids from *Sarcococca saligna* Against Acetyl- and Butyryl-Cholinesterase Enzyme, 9th International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 10-13.
- (53) M. N. Ghayur, M. Zain-ul-Sajadeen, A. H. Gilani, Zaheer-ul-Haq. S. K. Kalauni, A. Khalid, M.I. Choudhary, Atta-ur-Rahman, Antidiarrhoeal and Antisecretory Constituents in *Sarcococca saligna*, 9th International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 10-13.
- (54) Zaheer-ul-Haq, Atta-ur-Rahman, M.I. Choudhary, A. Khalid, S. Anjum and M.R. Khan, New Acetylcholinesterase Inhibitors from *Sarcococca saligna*, 7th Euroasia Conference on Chemical Sciences, Karachi, Pakistan, March 9-12. **[First prize winning poster]**
- (55) Khalid, M.I. Choudhary, M.K. Azim, S. Parveen, Zaheer-ul-Haq, Atta-ur-Rahman and S.A.M. Ayatollahi, Kinetic and Molecular Docking Studies on New Natural Cholinesterase Inhibitors, 2nd International & 12th National Chemistry Conference, Jamshoro, Pakistan, Feb. 4-6.
- (56) Atta-ur-Rahman, Zaheer-ul-Haq, A. Khalid, S. Anjum, M. R. Khan, and M. I. Choudhary, New Discoveries of Cholinesterase Inhibitors Studies from a Pakistani medicinal Plant, 2nd International and 12th National Chemistry Conference, University of Sindh, Jamshoro, Pakistan.
- (57) S. Anjum, Zaheer-ul-Haq, Atta-ur-Rahman, M. I. Choudhary and S. Aziz, Quantitative Estimation of Bilirubin by Hig Performance Liquid Chromatography (HPLC), HPLC2002, Montreal, Canada, June.
- (58) F. Feroz, Zaheer-ul-Haq, S. Anjum, Atta-ur-Rahman, and M.I. Choudhary, Synthetic Studies Towards Quinoxaline Derivatives and Rearrangement of Benzisoxazole System, 1st International and 11th National Chemistry Conference, Department of Chemistry, Peshawar, April 10 – 14, 2001.
- (59) Zaheer-ul-Haq, Atta-ur-Rahman, M.I. Choudhary, S. Anjum, A. Khalid and M.R. Khan, Bioassay-Guided Isolation of New Class of Acetylcholinesterase Inhibitors from *Sarcococca saligna*, 1st International and 11th National Chemistry Conference, Department of Chemistry, Peshawar, April 10 – 14, 2001

(60) Nuzhat Ahmed, Nazia Jalil, Zaheer-ul-Haq, Viqar-uddin Ahmad and Atta-ur-Rahman Commercially Important Products from Marine Bacteria: Marine Biotechnology, International Symposium on Marine Natural Products Chemistry, H.E.J. Research Institute of Chemistry University of Karachi.

(61) Zaheer-ul-Haq, Atta-ur-Rahman, M.I. Choudhary, S. Anjum and A. Khalid, Discovery of New Acetylcholinesterase Inhibitors from *Sarcococca saligna*, 8th International Symposium on Natural Product Chemistry, Karachi, Pakistan, Jan. 18-22.