

Curriculum Vitae and List of Publications

Dr. Umer Rashid

Associate Professor

**Department of Chemistry,
COMSATS University Islamabad,
Abbottabad Campus, PAKISTAN**

**American Chemical Society (ACS)
Reviewer Lab Graduate**

HEC approved supervisor

**Ex-Member American Chemical Society (ACS)
Ex-Member COMP-An ACS division of Computers in Chemistry
Member Chemical Society of Pakistan
Ex-IUPAC Affiliate Member**

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Area of Interest

(1) Design, synthesis and development of novel small-molecule drugs and multitarget inhibitors to treat human diseases including cancer (e.g. breast cancer), metabolic diseases (e.g. type II diabetes) and neurological diseases (e.g. Alzheimer's disease (AD)) using medicinal chemistry strategies in association with computer-aided rational drug design. (2) Application of new computational and informatics methods and tools for drug design and discovery. (3) Development of novel organic synthetic methodologies to achieve efficient drug synthesis and diversity-oriented synthesis.

Achievements

- ***Enlisted in 2023's World's Top 2% Scientist ranking released by Stanford University, USA***
- ***Nominated for the 2023 RSC Medicinal Chemistry Emerging Investigator Lectureship Award***
- ***Best Researcher Award, Department of Chemistry, COMSATS University, Abbottabad***

Personnel information

Father's Name:	Abdul Rashid
Date & Place of Birth	19 – 08 – 1973
NIC #	37405-1673741-3
Nationality	Pakistani
Marital status	Married
Mailing Address	Department of Chemistry, CUI, Abbottabad
Permanent Address	H. No. 39-D, Sector 4-B, Khayaban-e-Sirsyed, Rawalpindi, Pakistan
Phone No	+92 334 5171999
E – mail	umerrashid@cuiatd.edu.pk

Current Status

Associate Professor (Tenured)	Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, PAKISTAN
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Academics

Ph.D.	2011	Organic/Medicinal Chemistry from Quaid-i-Azam University, Islamabad
M.Sc	1997	Chemistry (Punjab University (G.C. Lahore)
B.Sc.	1994	Chemistry, Botany, Geography (Punjab University, Lahore)
F.Sc.	1991	Pre-Medical (Federal Government College for Men, H-9, Islamabad)
Matric	1989	Science (Federal Government High School NO.16, I-10/1, Islamabad)

Dissertations

Ph.D.	Dihydropyrimidines as potential drug candidates-Design, synthesis, bioevaluation and computational studies.
M.Sc.	Synthesis of Food dyes.

Post-Ph.D. Teaching/ Research Experiences (11 years)

1	Associate Professor (Tenured)	22-5-2023 to date	Department of Chemistry, COMSATS University Islamabad-Abbottabad Campus
2	Assistant Professor (<i>TTS</i>)	25-02-2016 to 21-5-2023	Department of Chemistry, COMSATS University Islamabad-Abbottabad Campus
3	Assistant Professor	24-08-2011 to 24-02-2016	Department of Chemistry, Hazara University, Mansehra

Research Projects

Project title	Amount in Rs (million)	Agency	Project ID No.	Status: Submitted / Approved / Completed
Tailoring the Substitution Pattern on Indanone and thiazolidinedione Core for Targeting Enzymes Associated with Alzheimer's Disease: Design, Synthesis and Biological Evaluations	8.68	HEC	20-14513/NRPU/R &D/HEC/2021 2021	Approved
Structure-based design and optimization of dihydropyrimidine-pteridine analogues as inhibitors of leishmania pteridine reductase and dihydrofolate reductase	5.2	HEC	5291/Federal/N RPU /R&D /HEC/2016	Completed
Design, synthesis and computational studies of dihydropyrimidine based urease and thymidine phosphorylase inhibitors	0.5	HEC	PM-IPFP/HRD/HEC /2011/346	Completed

Scholarships / Awards /Certificates

October 2023	Enlisted in 2023's World's Top 2% Scientist ranking released by Stanford University, USA.
December 2022	Nominated for the 2023 RSC Medicinal Chemistry Emerging Investigator Lectureship Award
October 2022	Best Researcher Award, Department of Chemistry, COMSATS University, Abbottabad
August 2022	Appreciation letter on Best Performance, COMSATS University, Abbottabad
2016-2018	Research Productivity Award
Feb. 1, 2010 – Jul. 31, 2010	HEC scholarship under International Research Support Initiative Program (IRSIP) for doing a part of Ph.D. research at Christian Doppler Laboratory for Microwave Chemistry (CDLMC), Karl-Franzens-University, Austria.
Sep. 1, 2009- Jan. 31, 2010, not availed	DAAD scholarship awarded for Germany, Rostock university
June 2004-May 2007	Merit Scholarship, Quaid-i-Azam University, Islamabad

Keynote / Invited speaker / Resource Person in Workshops/conferences/Symposium

February, 2023	Lecture on Rational Drug Design at University of Malakand, Chakdara
August 23, 2022	Keynote speaker at University of Wah, Wah Cantt.

August 17, 2022	University Of Gujrat
August 2, 2022	International Symposium on Computational Biology organized by Department of Biotechnology, COMSATS University, Abbottabad
July 2, 2022	International Symposium on Computational Chemistry, University of Agriculture, Faisalabad
November 28-29, 2018	Resource person, Molecular Modeling Workshop at Government Sadiq Women University, Bahawalpur
March 7-8, 2019	Resource person, Molecular Modelling Workshop, Department of Biotechnology, G.C University, Lahore
February 11-12, 2019	Speaker, First International Conference on Drug Discovery against Cancer and other diseases. University of Swabi

Membership of Learned Bodies

International	Member American Chemical Society (ACS)
	COMP-An ACS division of Computers in Chemistry
	IUPAC Affiliate member
National	Life Member, Chemical Society of Pakistan

Trainings / Courses

September 4-2019	ACS Lab Reviewer graduate
Feb. 3, 2010 – Jul. 25, 2010	Training in use of Microwave synthesizers (Biotage Initiator, CEM discover, Anton Paar microwave), Preparative chromatographic equipment (Biotage SP1), HPLC-UV, LCMS, GC-FID/GCMS in Christian Doppler Laboratory for Microwave Chemistry (CDLMC), Karl-Franzens-University, Austria

Co-curricular activities

March 2018 to Jan 2020	Secretary DARC, Department of Chemistry, COMSATS, Abbottabad
Sep. 2011 to Feb. 2016	Convener, Seminar Committee, Department of Chemistry, Hazara University, Mansehra
Jan. 2012-Dec.2012	Member Editorial board "Young Chemist

Editorial contribution / Manuscript Reviewer

1- Associate Editor , Frontiers in Chemistry, Medicinal and Pharmaceutical section: From September 1, 2022
2- Review Editor , Frontiers in Chemistry, Medicinal and Pharmaceutical section
3- Reviewer, Journal of Medicinal Chemistry (ACS)
4- Reviewer, Journal of Natural Product Chemistry (ACS)
5- Reviewer, European Journal of Medicinal Chemistry (Elsevier)
6- Reviewer, Journal of Enzyme Inhibition and Medicinal Chemistry (Taylor and Francis)
7- Reviewer, Future Medicinal Chemistry (Future Science UK)
8- Reviewer, Bioorganic Chemistry (Elsevier)
9- Reviewer, Journal of Molecular Structure (Elsevier)
10- Reviewer, Computational Biology and Chemistry (Elsevier)

Ph.D students Under Supervision

Safi Ullah	Department of Chemistry, COMSATS University, Abbottabad
Anees Saeed	Department of Chemistry, COMSATS University, Abbottabad
Sadia Shaheen	Department of Chemistry, COMSATS University, Abbottabad

Ph.D students Supervised / Co-Supervised

1	Muhammad Aamir Javed (Supervision)	2022	Tailoring the Substitution Pattern on Pyrimidine and Pyrrolidine for Targeting Enzymes Associated with Alzheimer's Disease: Design, Synthesis and Biological Evaluation	Department of Chemistry, COMSATS University, Abbottabad
2	Miss Aysha (Co-Supervision)	2022		University Of Gujrat
3	Sajjad Ahmad (Co-Supervision)	2021	Appraisal of anti-nociceptive potentials of the synthesized Michael adducts	Department of Pharmacy University of Malakand
4	Fatima Iftikhar (Co-Supervision)	2019	Design, Synthesis, Computational Studies and Bio-evaluation of Novel N-Heterocycles from Pyrimidine Scaffold	Department of Chemistry, Hazara University, Mansehra

M. Phil. / MS Students Supervised (At COMSATS, Abbottabad)

#	Student Name	Thesis Title	Status Registered/ Completed
1	Iqra Ejaz	Design and Synthesis of Pyrimidine Derivatives Targeting Estrogen Receptor-alpha for the Treatment of Breast Cancer	Completed
2	Ridha Jadoon	Design, Synthesis and Biological Evaluation of Thiazolidinedione Derivatives as Monoamine Oxidase-B Inhibitors	Completed
3	Saba Bibi	Design and Synthesis of 2-Aminothiazole-Based Multi-target Inhibitors to Tackle Cholinergic Deficit and Neuroinflammation in Alzheimer's Disease	Completed
4	Suleman Muraad	Design, Synthesis and Anti-cholinesterase Activity of Benzimidazole Derivatives	Completed
5	Rimsha Syed	Design, Synthesis and Molecular Modelling Study of Mefenamic Acid Analogs Endowed with Preferential COX-2 Inhibitory Activity	Completed
6	Sadia Khan	Tailoring the Substitution Pattern of Pyrrolidine-2,5-dione for Targeting Cyclooxygenase-2 Synthesis, Molecular Modeling, and Biological Evaluation as Anti-Inflammatory Agent	Completed
7	Nighat Ashraf	Design and Synthesis of Sulfonamide Derivatives as Selective COX-2 Inhibitors	Completed

	(CIIT/SP18-R06-021/ATD)		
8	Zeeshan Khan (CIIT/SP18-R06-015/ATD)	Synthesis of Gallic acid and Thiazolidine-2,4-dione Based α -Glucosidase and α -Amylase Inhibitors	Completed
9	Azmat Ullah (CIIT/FA18-RCM-030/ATD)	Structure-Based Design and Optimization of Mimics of Methotrexate as Potential Antileishmanial Agents	Completed
10	Flak Shair (CUI/FA18-RCM-031/ATD)	Design, Synthesis, In-vivo and In-silico Studies of Gabapentin Derivatives as Antiepileptic Agents	Completed
11	Haleema Bibi (FA18-R06-013)	Synthesis and DFT Studies of unsymmetrical Polymethine Cyanine Dyes Having Different N-Heterocyclic Rings	Completed
12	Sadia shaheen (FA18-R06-038)	Design and Synthesis of Thiourea Based Urease Inhibitors	Completed
13	Zaneb Kiran (CIIT/FA18-RCM-011/ATD)	Effect of Ligand Volume on AChE Inhibition: A Combined Synthetic and Computational Approach	Completed
14	Muhammad Bilal Tufail FA17-R06-016	Design, Synthesis and Pharmacological Evaluation of Progesterone and Pregnenolone Derivatives as Potent Anticancer Drugs	Completed
15	Memoona Pervaiz FA17-R06-039	Design and Synthesis of Piperazine and Piperidine Derivatives as Dual Binding Site Acetylcholinesterase Inhibitors	Completed
16	Sadaf Qureshi FA17-R06-028	Design, Synthesis and In Vitro Antibacterial Studies on Nitroimidazole Derivatives	Completed
17	Sana Malik FA17-R06-030	Theoretical Studies on Adsorption Ability of Zintl Ions for Hydrogen Storage	Completed
18	Mamoona FA17-R06-011	Identification of Diverse Scaffolds as Potential Inhibitors of Urease Using Matched Molecular Pairs and Scaffold Hopping Tools	Completed
19	Maria Bibi (FA16-R06-006)	Design, Synthesis and Docking Studies of Pyrimidines Derivatives as Potent Antileishmanial Drugs	Completed
20	Saba Tahir (FA16-R06-023)	Design, Synthesis and Anti-bacterial Studies of Piperazine Derivatives against Drug Resistant Bacteria	Completed
21	Muhammad Sajjad (SP17-R06-025)	Computer Guided Design and Synthesis of Dihydropyrimidine C-5 Acylhydroxamic Acid Derivatives as Potential Urease Inhibitors	Completed

22	Saba Tahir Tanoli (SP16-R06-007)	Computer assisted design, synthesis and bioevaluation of tricyclic fused ring system as dual binding site Acetylcholine esterase inhibitors	Completed
23	Maria Rasheed Khan (SP15-R06-012)	Design, Synthesis and Docking Studies of 1,2,4-Triazine Derived Schiff Base Metal Complexes as Potent Antileishmanial Drugs.	Completed

M. Phil. Supervised (At Hazara University, Mansehra)

1	Farhana Yaqoob	2013	Synthesis, C-6 modification and computational studies on dihydropyrimidine scaffold as thymidine phosphorylase inhibitors
2	Yousaf Ali	2013	Synthesis, C-5 modification and computational studies on Dihydropyrimidine scaffold as potent urease inhibitor
3	Riffat Sultana	2013	Synthesis, Molecular docking, structure–activity relationship and biological evaluation Dihydropyrimidines as antileishmanial agents
4	Syed Fahad Hassan (From University of Lahore)	2013	Medicinal Chemistry approaches in Drug Designing
5	M. Abeela (Co-Supervisor)	2013	Synthesis of imines prodrugs
6	Muhammad Jawad	2014	Design, Synthesis, Computational Studies and Bioevaluation Of Guanidine Containing Heterocycles
7	Farzana Bibi	2014	Computer Based Design and Synthesis of IL-2 Inhibitors
8	Afsheen Naz (Co-Supervisor)	2014	<i>Spectroscopic, DNA binding, molecular docking, partitioning and solubilization studies of new anticancer dihydropyrimidine derivatives</i>
9	Sufyan Ahmad	2014	<i>In silico</i> approach to design and synthesis of ligands for the treatment of Alzheimer’s disease

10	Ambreen Altaf	2015	2-Aminopyrimidines from chalcones and their tin (IV) complexes: Synthesis, antibacterial activity and computational studies
11	Kaniz Zahra	2015	Synthesis and drug loading on SiO ₂ coated Fe ₃ O ₄ nanoparticles for treatment of Alzheimer's disease
12	Atta Ullah	2015	Synthesis and antibacterial activity of some new amino acid derivatives
13	Muhammad Ayaz	2015	Structural modification and bioevaluation of some commercial drugs using bioisosteric approach
14	Saeed Anwar	2015	Thionation of carbonyl compounds using Lawesson's reagent: A comparative account of thermal, acoustic and microwave approach
15	Nasir Ud Din	2015	Computer based design and synthesis of novel potential antibacterials against highly resistant selected strains of microorganisms
16	Sadia Bibi	2015	Design and synthesis of cyclic thioureas as urease inhibitors
17	Waqas Ahmad (co-supervisor)	2015	Synthesis and antibacterial activity of some new trimethoprim derivatives
18	Sadia Farooq	2016	Synthesis and biological activity of anthranilic acid derivatives
19	Sundus Rasheed	2016	Synthesis, characterization, bioevaluation and computational studies on quinolone derivatives
20	Huzaifa	2016	Synthesis and drug loading on SiO ₂ coated Fe ₃ O ₄ nanoparticles in combating cancer
21	Ramzan Azhar	2016	Structural modification and bioevaluation of some commercial drugs containing carboxylic, amine and hydroxyl functionalities

External Examiner

SINES	NUST Islamabad
Department of Chemistry	Quaid-i-Azam University, Islamabad
Department of Chemistry	University of Gujrat, Gujrat
Department of Chemistry	Quaid-i-Azam University, Islamabad
Department of Chemistry	University of AJ&K, Muzaffarabad
Department of Chemistry	Hazara University, Mansehra
Department of Chemistry	Federal Urdu University, Karachi

Pre-Ph.D. Teaching/ Research & Industrial Experiences (12 years)

Visiting Ph.D Scholar	Feb. 2010 – July 2010	Christian Doppler Laboratory for Microwave Chemistry (CDLMC), Karl-Franzens University, Austria
Visiting Ph.D Scholar	July 2008- Sep. 2008	Dr. Punjwani Centre for Molecular Medicines & Drug Research (PCMD), Karachi, Pakistan
Plant Manager	Feb. - Aug. 2009	Neomedix Pharmaceuticals, Plot No. 5, N /5 National Industrial Zone, Rawat, Islamabad
Quality Control / Research & Development Manager	Aug 2005 – Jan 2009	Neomedix Pharmaceuticals, Plot No. 5, N /5 National Industrial Zone, Rawat, Islamabad
Analyst/Manager QC	Oct. 1997 to July. 2005	Islamabad Pharmaceutical Products, 34, Industrial Triangle, Islamabad.

List of Publications

Summary

Total Publications -----	152
Book Chapters -----	3
Review Articles-----	3
Research Articles ----	146
Total Impact Factor -----	622

Citations 3581

h-index = 35

i10-index = 90

Book Chapters		
N o.	Year	Complete Description
1.	2022	Nishant Rai, Pramond Rawat, Rakesh K Bachheti, Navin Kumar, Abdul Rauf, Umer Rashid , Vijay Jyoti Kumar, Tanmay Sarkar, Raffaele Pezzani. Sustainable uses of medicinal plants and prospects; Chapter title, Characterization and docking studies of immunomodulatory active compounds from Rhododendron arboreum leaves. CRC / Taylor and Francis Books (Accepted 2022)
2.	2020	Muhammad Naveed Anjum, Shoaib Ahmad Malik, Choudhary Haseeb Bilal, Umer Rashid, Muhammad Nasif, Khalid Mahmood Zia. Chapter 13 - Polyhydroxyalkanoates-based bionanocomposites. Bionanocomposites; Green Synthesis and Applications: Micro and Nano Technologies. 2020, Pages 321-333 https://www.sciencedirect.com/science/article/pii/B9780128167519000131#:~:text=Abstract,and%20bacteria%20and%20fermentation%20conditions.
3.	2014	Umer Rashid , Farzana Latif Ansari. <i>Challenges in designing therapeutic agents for treating Alzheimer's disease-From serendipity to rationality</i> . Drug Design and Discovery in Alzheimer's Disease (Elsevier), (2014), vol. 6 Chapter 2, pp 40-141 ISBN-13: 978-0128039595, ISBN-10: 0128039590

Research Articles (Published)			
2024			
1.	2024	Bushra Mobeen a, Muhammad Shah a, Hafiz Muzzammel Rehman b, Muhammad Saeed Jan c, Umer Rashid. Discovery of the selective and nanomolar inhibitor of DPP-4 more potent than sitagliptin by structure-guided rational design. European Journal of Medicinal Chemistry 279 (2024) 116834	6.0
2.	2024	Gauhar Rehman a, Ilman Khan a, Abdur Rauf b, Umer Rashid c, Arshma Siddique c, Syed Muhammad Mukarram Shah d, Zuneera Akram e, Najla AlMasoud f, Taghrid S. Alomar f, Zafar Ali Shah b, Giovanni Ribaud. Antidiabetic Properties of Caffeoylmalic Acid, a Bioactive Natural Compound Isolated from Urtica dioica. Fitoterapia. 176, (2024), 106024	3.4

3.	2024	Ayesha Tahir, Bushra Mobeen, Fahad Hussain, Abdul Sadiq and <u>Umer Rashid</u> . Pregnenolone derivatives for the treatment of Alzheimer's disease: synthesis, and in vitro inhibition of amyloid b1–42 peptide aggregation, acetylcholinesterase and carbonic anhydrase-II. RSC Adv., 2024, 14, 14742	3.9
4.	2024	Gowhar Ali, Farrah Deeba, Umer Rashid, Aman Ullah, Hammad Ullah, Inayat Ali Khan, Syed Ishtiaq Khan, Amin Badshah, Muhammad Arif Khan, Muhammad Ayaz g, Maria Daglia. In vivo effects of a selected thiourea derivative 1-(2-chlorobenzoyl)-3-(2,3-dichloro phenyl) against nociception, inflammation and gastric ulcerogenicity: Biochemical, histopathological and in silico approaches Biomedicine and Phrmacotherapy. 174 (2024) 116544	7.5
5.	2024	Mater H. Mahnashi, Umer Rashid*, Hassan Hussain Almasoudi, Mohammed H. Nahari, Imran Ahmad, Abdulkarim S. Binshaya, Osama Abdulaziz, Meshari A. Alsuwat, Muhammad Saeed Jan, and Abdul Sadiq. Modification of 4-(4-chlorothiophen-2-yl)thiazol-2-amine derivatives for the treatment of analgesia and inflammation: synthesis and in vitro, in vivo, and in silico studies Frontiers in Pharmacology (Accepted) DOI 10.3389/fphar.2024.1366695	5.6
6.	2024	Muhammad Imran Qayyum, Sami Ullah, <u>Umer Rashid</u> , Abdul Sadiq, Mater H. Mahnashi, Saif Ullah Khan Khalil, Muhammad Masoom Akhtar. N -phenyl and N-benzyl substituted succinimides: Preclinical evaluation for their antihypertensive effect and underlying mechanism. European Journal of Pharmacology, 964 (2024) 176195	5.0
7.	2024	Fahad Hussain,a Ayesha Tahir, Muhammad Saeed Jan, Noor Fatima, Abdul Sadiq and Umer Rashid. Exploitation of the multitarget role of new ferulic and gallic acid derivatives in oxidative stress related Alzheimer's disease therapies: design, synthesis and bioevaluation. RSC Adv., 2024, 14, 10304	3.9
8.	2024	Abdur Rauf*, Umer Rashid, Zuneera Akram, Momina Ghafoor, Naveed Muhammad, Najla Al Masoud, Taghrid S. Alomar, Saima Naz and Marcello Iriti. In vitro and in silico antiproliferative potential of isolated flavonoids constitutes from Pistacia integerrima. Z. Naturforsch. 2024; aop	1.8

9.	2024	Abdur Rauf, Umer Rashid, Zafar Ali Shah, Anees Ahmed Khalil, Muhammad Shah, Tabussam Tufail, Gauhar Rehman, Abdur Rahman, Saima Naz, Abdulrahman Alsahammari, Metab Alharbi, Abdulmajeed AL-Shahrani and Dorota Formanowicz. Anti-Inflammatory and Anti-Diabetic Properties of Indanone Derivative Isolated from <i>Fernandoa adenophylla</i> in vitro and in silico Studies. Scientific Reports (Nature) Accepted 15-4-2024	4.6
10.		Abdur Rauf, Aniqat Attab, Umer Rashid, Yahya S. Al-Awthan, Omar S. Bahattab, Zafar Ali Shah, Muhammad Shah, Saima Naz, Zubair Ahmad, Sami Siraj, Ishaq Khan, Hassan A. Hemeg. Anticancer Potential and In Silico computational studies of bioactive secondary metabolites isolated from <i>Heterophragma adenophyllum</i> (Wall. ex G. Don) Steenis. Minerva Biotechnol Biomol (Accepted)	1.0
2023			
11.	2023	Abdur Rauf, Bassam Oudh Aljohny, Umer Rashid , Yasir Anwar, Zafar Ali Shah, Naveed Muhammad, Anees Ahmed Khalil, Ahood Khalid, Gauhar Rehman. In vitro anti-inflammatory, antidiabetic, antibacterial, and in silico studies of Ferruginan A isolated from <i>Olea ferruginea</i> Royle (Oleaceae). Saudi Pharmaceutical Journal 31 (2023) 101868	4.1
12.	2023	Hasnain Mehmood, Tashfeen Akhtar, Muhammad Haroon, Muhammad, Shah, Umer Rashid & Simon Woodward. Synthesis of hydrazinylthiazole carboxylates: a mechanistic approach for treatment of diabetes and its complications. Future Medicinal Chemistry Volume 15, 2023 - Issue 13 , 1-17	3.2
13.	2023	Kiran Shahzadi, Syed Majid Bukhari, Asma Zaidi, Tanveer A. Wani, Muhammad Saeed Jan, Seema Zargar, Umer Rashid , Umar Farooq, Aneela Khushal and Sara Khan. Novel Coumarin Derivatives as Potential Urease Inhibitors for Kidney Stone Prevention and Antiulcer Therapy: From Synthesis to In Vivo Evaluation. Pharmaceuticals 2023, 16, 1552.	4.6
14.	2023	Zainab Bibi, Irfa Asghar, Naeem Mahmood Ashraf, Iftikhar Zeb, Umer Rashid , Arslan Hamid, Maria Kanwal Ali, Ashraf Atef Hatamleh, Munirah Abdullah Al-Dosary, Raza Ahmad and Muhammad Ali.	4.6

		Prediction of Phytochemicals for Their Potential to Inhibit New Delhi Metallo -Lactamase (NDM-1). Pharmaceuticals 2023, 16, 1404.	
15.	2023	Abdur Rauf, Umer Rashid , Aniqā Atta, Ishaq Khan, Zafar Ali Shah, Bushra Mobeen, Aneela Javed, Taghrid S. Alomar, Najla Almasoud, Saima Naz, Zubair Ahmad, Giovanni Ribaud. Antiproliferative Activity of Lignans from Olea ferruginea: In Vitro Evidence Supported by Docking Studies. Front. Biosci. (Landmark Ed) 2023; 28(9): 216	3.1
16.	2023	Taghrid S AlOmar, Abdur Rauf, Umer Rashid , Sehrish Sarfaraz, Khurshid Ayub, Fahad Hussain, Najla Almasoud, Abdulaziz S AlOmar, Gauhar Rehman, Zubair Ahmad, Naveed Muhammad, Zafar Ali Shah. Molecular docking, DFT studies, and anti-inflammatory evaluation of peshawaraquinone isolated from Fernandoa adenophylla. J Biomol Struct Dyn. 2023:1-13.	4.4
17.	2023	Sehrish Sarfaraz, Muhammad Yar, Ajaz Hussain, Ahmed Lakhani, Adnan Gulzar, Muhammad Ans, Umer Rashid , Masroor Hussain, Shabbir Muhammad, Imene Bayach*, Nadeem S. Sheikh* and Khurshid Ayub. Metallofullerenes as robust single atom catalysts for adsorption and dissociation of hydrogen molecule: A density functional study. Accepted ACS Omega (31-8-23)	4.1
18.	2023	Waqas Alam, Haroon Khan, Muhammad Saeed, Umer Rashid , Ali Abusharha, Maria Daglia. Synthesis, in-vitro inhibition of cyclooxygenases and in-silico studies of New Isoxazole Derivatives. Frontiers in Chemistry	5.5 2296-2646
19.	2023	Muhammad Shah, Muhammad Saeed Jan, Abdul Sadiq, Sara Khan, Umer Rashid . SAR and lead optimization of (Z)-5-(4-hydroxy-3-methoxybenzylidene)-3-(2-morpholinoacetyl)thiazolidine-2,4-dione as a potential multi-target antidiabetic agent. European Journal of Medicinal Chemistry 258 (2023) 115591	6.7 0223-5234
20.	2023	Qarib Ullah, Zarshad Ali, Umer Rashid , Gowhar Ali,* Nisar Ahmad, Rasool Khan, Sami Ullah, Muhammad Ayaz, and H C Ananda Murthy. Involvement of the Opioidergic Mechanism in the Analgesic Potential of a Novel Indazolone Derivative: Efficacy in the Management of Pain, Neuropathy, and Inflammation Using In Vivo and In Silico Approaches. ACS Omega 2023, 8, 25, 22809–22819	4.1 2210-7177



21.	2023	Aneela Gohar, Gowhar Ali, Umer Rashid , Khalid Rauf, Mehreen Arif, Muhammad Sona Khan, Yasser MSA Alkahramaan, Robert DE Sewell. Effect of Gabapentin-Fluoxetine Derivative GBP1F in a Murine Model of Depression, Anxiety and Cognition. Drug Design, Development and Therapy 2023;17 1793–1803	4.319 1177-8881
22.	2023	Abdur Rauf, Umer Rashid , Abdullah Muhammad Shbeer, Mohammed Al-Ghorbani, Naveed Muhammad, Anees Ahmed Khalil, Humaira Naz, Rohit Sharma & Giovanni Ribaudo. Flavonoids from Pistacia chinensis subsp. integerrima with leishmanicidal activity: computational and experimental evidence. Natural Product Research (Accepted)	2.488 1478-6419
23.	2023	Haleema Ali, Rasool Khan, Xiandao Pan, Farzana Shaheen, Almas Jabeen, Abdur Rauf, Muhammad Shah, Umer Rashid , Yahya S. Al-Awthan, Omar S. Bahattab, Mohammed A. Al-Duais, Mohammad S. Mubarak. Synthesis, characterization, anti-cancer, anti-inflammatory activities, and docking studies of 3, 5-disubstituted thiadiazine-2-thiones. Green Processing and Synthesis 2023; 12: 20228136	3.970 2191-9542
24.	2023	Abdur Rauf , Umer Rashid , Zafar Ali Shah, Gauhar Rehman, Kashif Bashir, Johar Jamil, - Iftikhar, Abdur Rahman, Abdulrahman Alsahammari, Metab Alharbi, Abdulmajeed Al-Shahrani, Giovanni Ribaudo. Anti-inflammatory and Anti-diabetic Activity of Ferruginan, a Natural Compound from Olea ferruginea. Processes (MDPI) 2023, 11, 545.	3.352
25.	2023	Imene Bayach, Atazaz Ahsin, Safi Ullah Majid, Umer Rashid , Nadeem S. Sheikh, and Khurshid Ayub. Geometric, electronic, and optoelectronic properties of carbon-2 based polynuclear $C3O[C(CN)2]2M3$ (where $M=Li, Na, \text{ and } K$) 3 clusters; A DFT study. Molecules 2023, 28(4), 1827	4.927
26.	2023	Mater H. Mahnashi , Waqas Alam , Mohammed A. Huneif, Alqahtani Abdulwahab, Mohammed Jamaan Alzahrani, Khaled S. Alshaibari, Umer Rashid , Abdul Sadiq, and Muhammad Saeed Jan. Exploration of Succinimide Derivative as a Multi-Target, Anti-Diabetic Agent: In Vitro and In Vivo Approaches. Molecules, 2023, 28, 1589	4.927
27.	2023	Mohammed A. Huneif , Mater H. Mahnashi, Muhammad Saeed Jan, Muhammad Shah, Sultan A. Almedhesh, Seham M. Alqahtani,	4.927


		Mohammad Jamaan Alzahrani, Muhammad Ayaz, Farhat Ullah, Umer Rashid and Abdul Sadiq. New Succinimide–Thiazolidinedione Hybrids as Multitarget Antidiabetic Agents: Design, Synthesis, Bioevaluation, and Molecular Modelling Studies. <i>Molecules</i> 2023, 28, 1207.	
28.	2023	Nargis Sultana, Muhammad Sarfraz, Sidra Akram, Umer Rashid , Syed Ali Raza Naqvi, Muhammad Tariq, Khalid Mahmood Zia, Muhammad Ramzan Saeed Ashraf Janjua. Reactivity of 2,2-Disubstituted Quinazolinone Towards Electrophilic Substitution: First In-Silico Design to Verify Experimental Evidence of Quinazolinone-based New Organic Compounds. <i>Journal of Physical Organic Chemistry</i> , (Accepted) 20 January 2023	2.155 0894-3230
29.	2023	Bushra Ansari, Haroon Khan, Muhammad Saeed Jan, Khalaf F. Alsharif, Khalid J. Alzahrani, Umer Rashid , and Abdul Saboor Pirzada. Synthesis, Characterization, and Pharmacokinetic Studies of Thiazolidine-2,4-Dione Derivatives. <i>Journal of Chemistry</i> , Volume 2023, Article ID 9462176	3.241 2090-9063
30.	2023	Muhammad Aamir Javed, Muhammad Saeed Jan, Abdullah M. Shbeer, Mohammed Al-Ghorbani, Abdur Rauf, Polrat Wilairatana, Abdul Mannan, Abdul Sadiq, Umar Farooq, Umer Rashid. Evaluation of pyrimidine / pyrrolidine-sertraline based hybrids as multitarget anti-Alzheimer agents: In-vitro, in-vivo, and computational studies. <i>Biomedicine & Pharmacotherapy</i> 159 (2023) 114239	7.410 0753-3322
31.	2023	Muhammad Imran Qayyum, Sami Ullah, Obaidullah, Umer Rashid, Mater H. Mahnashi, Mohammed Merae Alshahrani, Amer Al Ali, Abdulaziz Asiri, Ahmed Abdullah Al Awadh, Osama M. Alshehri, Abdul Sadiq. Design, synthesis and preclinical evaluations of (s)-2-((s)-1-benzyl-2,5-dioxopyrrolidin-3-yl)-3-(4-isopropylphenyl)-2-methyl propanal (succ-5) as cardioprotective, hepatoprotective and lipid lowering molecule. in-vivo and in-silico approaches. <i>Arabian Journal of Chemistry</i> , Volume 16, Issue 2, 104504	6.212 1878-5352
32.	2023	Paras Nath Yadav, Shivani Sharma, Motee Lal Sharma, Abdur Rauf, Umer Rahid and Yuba Raj, Pokharel. Platinum (II) Complexes of 3-Hydroxypyridine-2-Carboxaldehyde, N(4)-Methyl and N(4)-Pyrrolidinyl Thiosemicarbazones: Synthesis, Characterization, and Primary Anticancer Screening against HeLa Cells, and Molecular Docking. <i>Current Indian Science</i>	1.169

2022

33.	2022	Ridha Jadoon, Muhammad Aamir Javed, Muhammad Saeed Jan ,Ikram Muhammad,Mater H. Mahnashi ,Abdul Sadiq ,Muhammad Shahid, <u>Umer Rashid</u> . Design, synthesis, in-vitro, in-vivo and ex-vivo pharmacology of thiazolidine-2,4-dione derivatives as selective and reversible monoamine oxidase-B inhibitors, Bioorganic & Medicinal Chemistry Letters, 76, 2022, 128994	2.94 0960-894X
34.	2022	Hassan A. Hemeg, Abdur Rauf , <u>Umer Rashid</u> , Naveed Muhammad, Yahya S. Al-Awthan , Omar S. Bahattab , Mohammed A. Al-Duais, Syed Uzair Ali Shah, and Rohit Sharma. In-Vitro Leishmanicidal Activity and Molecular Docking Simulations of a Flavonoid Isolated from Pistacia integerrima Stew ex Brandis. Journal of Food Quality, Volume 2022 Article ID 6003869	3.200 0146-9428
35.	2022	Muhammad Imran Qayyum, Sami Ullah, <u>Umer Rashid</u> , Abdul Sadiq, Obaid Ullah, Mater H Mahnashi, Osama M. Alshehri, Mohammed M. Jalal, KhalidJ. Alzahrani, Ibrahim F. Halawani. Synthesis, molecular docking and preclinical evaluation of new succinimide derivative for cardioprotective, hepatoprotective and lipid lowering effects. Molecules 2022, 27(19), 6199;	4.927 1420-3049
36.	2022	Sana Shamim, Somia Gul, Abdur Rauf, <u>Umer Rashid</u> , Ajmal Khan, Rafat Amin, Faiza Akhtar. Gemifloxacin-transition metal complexes as therapeutic candidates: antimicrobial, antifungal, anti-enzymatic and docking studies of newly synthesized complexes. Heliyon 2022;8(8):e10378.	3.776 2405-8440
37.	2022	Hassan A. Hemeg, Abdur Rauf, <u>Umer Rashid</u> , Naveed Muhammad, Yahya S. Al-Awthan, Omar S. Bahattab, Mohammed A. Al-Duais, Syed Uzair Ali Shah. In vitro α -glycosidase inhibition and in silico studies of Flavonoids isolated from Pistacia integerrima Stew ex Brandis. BioMed Research International, Volume 2022, Article ID 9636436, 6 pages	3.246 2314-6133
38.	2022	Muhammad Aamir Javed, Saba Bibi, Muhammad Saeed Jan, Muhammad Ikram, Asma Zaidi, Umar Farooq, Abdul Sadiq and <u>Umer Rashid</u> . Diclofenac derivatives as concomitant inhibitors of cholinesterase, monoamine oxidase, cyclooxygenase-2 and 5-lipoxygenase for the treatment of Alzheimer's disease: Synthesis,	4.036 2046-2069

		pharmacology, toxicity and docking studies. RSC Advances 2022, 12, 22503–22517	
39.	2022	Wajeeha Waseem, Fareeha Anwar, Uzma Saleem, Bashir Ahmad, Rehman Zafar, Asifa Anwar, Muhammad Saeed Jan, Umer Rashid , Abdul Sadiq, Tariq Ismail. Prospective Evaluation of Amide Based Zinc Scaffold as Anti-Alzheimer Agent: In-Vitro, In-Vivo and Computational Studies. ACS Omega 2022, 7, 26723–26737	4.132
40.	2022	Wahid Zada, Jonathan W VanRyzin, Miguel Perez-Pouchoulen, Samantha L Baglot, Matthew N Hill, Ghulam Abbas, Sarah M. Clark, Umer Rashid, Margaret M McCarthy, Abdul Mannan. Fatty acid amide hydrolase inhibition and N-arachidonoyl ethanolamine modulation by isoflavonoids: A novel target for upcoming antidepressants. Pharmacology Research & Perspectives 2022 10(5):e00999	2.963 2052-1707
41.	2022	Fawad Mahmood, Jamshaid Ali Khan, Mater H. Mahnashi, Muhammad Saeed Jan, Muhammad Aamir Javed, Umer Rashid, Abdul Sadiq, Syed Shams ul Hassan, Simona Bungau. Anti-Inflammatory, Analgesic and Antioxidant Potential of New (2S,3S)-2-(4-isopropylbenzyl)-2-methyl-4-nitro-3-phenylbutanals and Their Corresponding Carboxylic Acids through In Vitro, In Silico and In Vivo Studies, Molecules 2022, 27, 4068.	4.927
42.	2022	Bandar A. Alyami, Iqra Ejaz, Mater H. Mahnashi, Yahya S. Alqahtani, Ali O. Alqarni, Muhammad Saeed Jan, Abdul Sadiq, Umer Rashid. Design, synthesis, antiproliferative activity, estrogen receptors binding affinity of C-3 pregnenolone-dihydropyrimidine derivatives for the treatment of breast cancer. Steroids 185 (2022) 109059	2.76 0039-128X
43.	2022	Zainab Ayaz, Bibi Zainab, Umer Rashid, Noura M. Darwish, Mansour K. Gatasheh, and Arshad Mehmood Abbasi. In Silico Screening of Synthetic and Natural Compounds to Inhibit the Binding Capacity of Heavy Metal Compounds against EGFR Protein of Lung Cancer. BioMed Research International. Volume 2022, Article ID 2941962, 12 pages	3.246
44.	2022	Abdul Sadiq; Mater H. Mahnashi; Umer Rashid; Muhammad Saeed Jan; Mohammed Abdulrahman Alshahrani; Mohammed A. Huneif; 3-(((1S,3S)-3-((R)-Hydroxy(4-(trifluoromethyl)phenyl)methyl)-4-oxocyclohexyl)methyl)pentane-2,4-dione: Design and Synthesis of	4.927


		New Stereo pure Multi-Target Antidiabetic Agent. <i>Molecules</i> 2022, 27(10), 3265	
45.	2022	Abdullah S. M. Aljohani; Fahad A. Alhumaydhi; Abdur Rauf; Essam M. Hamad; Umer Rashid. In Vivo and in vitro biological evaluation and molecular docking studies of compound isolated from <i>Micromeria biflora</i> (Buch. Ham. ex D.Don) Benth. <i>Molecules</i> 2022, 27(11), 3377	4.927
46.	2022	Bilal Ahmad Khan , Syeda Shamila Hamdani , Muhammad Naeem Ahmed , Umer Rashid , Shahid Hameed , Mahmoud A.A. Ibrahim , Jamshaid Iqbal , Cristian C. Granados , Mario A. Macías. Design, Synthesis, Crystal Structures, Computational Studies, in vitro and in silico Monoamine Oxidase-A&B Inhibitory Activity of Two Novel S-Benzyl Dithiocarbamates. <i>Journal of Molecular Structure</i> 1265, 2022, 133317	3.841 0022-2860
47.	2022	Mohammed A. Huneif, Dhafer Batti Alshehri, Khaled S. Alshaibar, Mayasa Z. Dammaj, Mater H. Mahnashi, Safi Ullah Majid, Muhammad Aamir Javed, Sajjad Ahmad, Umer Rashid, Abdul Sadiq. Design, synthesis and bioevaluation of new vanillin hybrid as multitarget inhibitor of α -glucosidase, α -amylase, PTP-1B and DPP4 for the treatment of type-II diabetes. <i>Biomedicine & Pharmacotherapy</i> 150 (2022) 113038	7.419
48.	2022	Iqra Ejaz, Muhammad Aamir Javed, Muhammad Saeed Jan, Muhammad Ikram, Abdul Sadiq, Sajjad Ahmad, Umer Rashid. Rational design, synthesis, antiproliferative activity against MCF-7, MDA-MB-231 cells, estrogen receptors binding affinity, and computational study of indenopyrimidine-2,5-dione analogs for the treatment of breast cancer. <i>Bioorganic and Medicinal Chemistry Letter</i> Volume 64, 15 May 2022, 128668	2.94
49.	2022	Muhammad Shahid Nadeem, Jalaluddin Azam Khan, Imran Kazmi, <u>Umer Rashid</u>  . Design, synthesis and bioevaluation of indole core containing 2-arylidine derivatives of thiazolopyrimidine as multitarget inhibitors of cholinesterases and monoamine oxidase A/B for the treatment of Alzheimer disease. <i>ACS Omega</i> , 2022, 7, 11, 9369–9379	4.132
50.	2022	Mater H. Mahnashi, Bandar A. Alyami, Yahya S. Alqahtani, Ali O. Alqarni, Muhammad Saeed Jan, Muhammad Ayaz, Farhat Ullah, <u>Umer Rashid</u>  and Abdul Sadiq. Molecular Docking Supported	0.698

		Observed Changes in Anticholinesterase, Antioxidant and α -Glucosidase Inhibitions upon the Bromination of Benzene Sulfonamide. J Chem. Soc. Pak. 44 (2022) 69	
51.	2022	Mater H. Mahnashi, Bandar A. Alyami, Yahya S. Alqahtani, Ali O. Alqarni, Muhammad Saeed Jan, Fida Hussain, Rehman Zafar, Umer Rashid  , Muhammad Abbas, Muhammad Tariq, and Abdul SadiqAntioxidant molecules isolated from edible prostrate knotweed: Rational derivatization to produce more potent molecules. Oxidative Medicine and Cellular Longevity. Volume 2022, Article ID 3127480, 15 pages	7.31 1942-0994
52.	2022	Aishaa, Muhammad Asam Razaa, Umme Farwa, Umer Rashid, Jan K. Maurin, Armand Budzianowski. Synthesis, single crystal, in-silico and in-vitro assessment of the thiazolidinones. J. Mol. Str. 1255 (2022) 132384	3.841
53.	2022	Mehreen Ghias, Muhammad Naeem Ahmed, Bakhtawar Sajjad, Mahmoud A .A . Ibrahim, Umer Rashid, Syed Wadood Ali Shah, Mohammad Shoaib, Murtaza Madni, Muhammad Nawaz Tahir, Mario A. Macías 1-Hydroxynaphthalene-4-trifluoromethylphenyl chalcone and 3-hydroxy-4-trifluoromethylphenyl flavone: A combined experimental, structural, in vitro AChE, BChE and in silico studies. J. Mol. Str. 1253 (2022) 132253	3.841
54.	2022	Zafar Ali Shah, Adil A. H. Mujawah , Irfan Ullah, Abdur Rauf, Umer Rashid , Anees Ahmed Khalil ,4 Syed Muhammad Mukarram Shah,5 Aini Pervaiz, Farzana Shaheen, Yahya S. Al-Awthan, Muhammad Nasimullah Qureshi, Mohammed A. Al-Duais, Omar Bahattab, Zainab M. Almarhoon , Yahia N. Mabkhot , and Mohammad S. Mubarak. Antioxidant and Cytotoxic Activity of a New Ferruginan A from Olea ferruginea: In Vitro and In Silico Studies. Oxidative Medicine and Cellular Longevity Volume 2022, Article ID 8519250, 7	7.31
2021			
55.	2021	Muhammad Shahid Nadeem, Jalaluddin Azam Khan, Umer Rashid. Fluoxetine and Sertraline based Multitarget Inhibitors of Cholinesterases and Monoamine Oxidase-A/B for the treatment of Alzheimer's Disease: Synthesis, Pharmacology and Molecular	6.953 0141-8130

		Modeling Studies. International Journal of Biological Macromolecules. 193 (2021) 19–26	
56.	2021	Muhammad Aamir Javed, Nighat Ashraf, Muhammad Saeed Jan, Mater H. Mahnashi, Yahya S. Alqahtani, Bandar A. Alyami, Ali O. Alqarni, Yahya I. Asiri, Muhammad Ikram, Abdul Sadiq, Umer Rashid . Structural modification, in-vitro, in-vivo, ex-vivo and in-silico exploration of pyrimidine and pyrrolidine cores for targeting enzymes associated with neuroinflammation and cholinergic deficit in Alzheimer's disease. ACS Chemical Neuroscience, 2021, 12, 21, 4123-4143	5.78 1948-7193
57.	2021	Mater H. Mahnashi, Yahya S. Alqahtani, Ali O. Alqarni, Bandar A. Alyami, Muhammad Saeed Jan, Muhammad Ayaz, Farhat Ullah, Umer Rashid, Abdul Sadiq. Crude extract and isolated bioactive compounds from <i>Notholirion thomsonianum</i> (Royale) Stapf as multitargets antidiabetic agents: In-vitro and molecular docking approaches. BMC Complement Med Ther. 21, 270	2.838 2662-7671
58.	2021	Mater H. Mahnashi, Bandar A. Alyami, Yahya S. Alqahtani, Ali O. Alqarni, Muhammad Saeed Jan, Muhammad Ayaz, Farhat Ullah, Muhammad Shahid, Umer Rashid and Abdul Sadiq. Neuroprotective potentials of selected natural edible oils using enzyme inhibitory, kinetic and simulation approaches. BMC Complement Med. Ther. (2021) 21:248	2.838
59.	2021	Ala Ud Din, Maria Khan, Muhammad Zahir Shah, Abdur Rauf, Umer Rashid, Anees Ahmed Khalil, Khair Zaman, Yahya S. Al-Awthan, Mohammed A. Al-Duais, Omar Bahattab, Adil A.H. Mujawah, Naveed Muhammad. Anti-diabetic activity of Ficusonolide; A triterpene lactone from <i>Ficus foveolata</i> (Wall. ex Miq.): In-vitro, in-vivo and in-silico approaches. ACS Omega 6, 41, 27351–27357	4.132
60.	2021	Bibi Zainab, Zainab Ayaz, Umer Rashid, Dunia A. Al Farraj, Roua M. Alkufeidy, Fatmah S. AlQahtany, Reem M. Aljowaie, and Arshad Mehmood Abbasi. Role of persistent organic pollutants in Breast Cancer Progression and Identification of Estrogen Receptor Alpha Inhibitors using In-silico Mining and Drug-drug Interaction Network Approaches. Biology (MDPI) 10 (2021) 681	5.168 2079-7737
61.	2021	Abdur Rauf, Umer Rashid , Anees Ahmed Khalil, Shahid Ali Khan, Sirajudheen Anwar, Ahmed Alafnan, Kannan RR Rengasamy.	3.111


		Docking-based virtual screening and identification of potential COVID-19 main protease inhibitors from brown algae. South African Journal of Botany, 2021, 143: 428–434	0254-6299
62.	2021	Yahya S., Al-Awthan, Omar Bahattab, Zafar Ali Shah, Saud Bawazeer, Mohammad Ali Shariati, Mohamad Fawzi Mahomoodally, Sirajudheen Anwar, Kannan RR Rengasamy, Umer Rashid , Abdur Rauf . Potent urease inhibition and in silico docking study of four secondary metabolites isolated from <i>Heterophragma adenophyllum</i> Seem. South African Journal of Botany, 2021, 142, 201-205	3.111
63.	2021	Mohammed Mansour Quradha, Rasool Khan, Achyut Adhikari, Abdur Rauf, Umer Rashid, Sami Bawazeer, Yahya S. Al-Awthan, Omar Bahattab, Mohammad S. Mubarak. Isolation, biological evaluation and molecular docking studies of compounds from <i>Sophora mollis</i> (Royle) Graham ex Baker. ACS Omega 2021, 6, 15911–15919	4.132
64.	2021	Shehla Parveena, Hammad Saleemb, Muhammad Sarfraz, Umair Khurshid, Maroof Habib, Mamona Nazir, Naseem Akhtar, Faiz-Ul-Hassan Nasim, Umer Rashid, Ghayoor Abbas Chotana. Phytochemical profiling, In vitro antioxidant and identification of urease inhibitory metabolites from <i>Erythrina suberosa</i> flowers by GC-MS analysis and docking studies. South African Journal of Botany, 2021, 143, 422-427	3.111
65.	2021	Fahad A. Alhumaydhi, Abdur Rauf#, Umer Rashid, Saud Bawazeer, Khalid Khan, Mohammad Mubarak, Abdullah S. M. Aljohani, Haroon Khan, Gaber El-Saber Batiha, Mohamed A. El-Esawi, Abhay P. Mishra. In vivo and in silico studies of flavonoids isolated from <i>Pistacia integerrima</i> as potential anti-diarrheal agents. ACS Omega. 2021, 6, 15617–15624	4.132
66.	2021	Yahya S. Al-Awthan, Abdur Rauf, Umer Rashid, Saima Naz, Sami Bawazeer, Omar Bahattab, Saud Bawazeer, Naveed Muhammad, Hafiz Ansar Rasul Suleria, Gaber El-Saber Batiha, Mohammad Ali Shariati, Marina Derkho. Sedative-hypnotic effect and in silico study of dinaphthodiospyrrols isolated from <i>Diospyros lotus</i> Linn. Biomedicine & Pharmacotherapy. Volume 140, 2021, 111745	7.419
67.	2021	Abdul Sadiq, Mater H. Mahnashi, Bandar A. Alyami, Yahya S. Alqahtani, Ali O. Alqarni, Umer Rashid . Tailoring the Substitution	5.307

		Pattern of Pyrrolidine-2,5-dione for Discovery of new structural template for dual COX / LOX inhibition. Bioorganic Chemistry. Volume 112, 2021, 104969	0045-2068
68.	2021	Jawad Khan, Gowhar Ali, Umer Rashid, Rasool Khan, Muhammad Saeed Jan, Rahim Ullah, Sajjad Ahmad, Sumra Wajid Abbasi, Atif Ali Khan Khalil, Robert D.E. Sewell. Mechanistic evaluation of a novel cyclohexenone derivative's functionality against nociception and inflammation: An in-vitro, in-vivo and in-silico approach. European Journal of Pharmacology, 902 (2021) 174091	5.195 0014-2999
69.	2021	Mater H. Mahnashi, Bandar A. Alyami, Yahya S. Alqahtani, Muhammad Saeed Jan, Umer Rashid, Abdul Sadiq. Phytochemical profiling of bioactive compounds, anti-inflammatory and analgesic potentials of <i>Habenaria digitata</i> Lindl.: Molecular docking based synergistic effect of the identified compounds. Journal of Ethnopharmacology. 273, 2021, 113976	5.195 1872-7573
70.	2021	Sajjad Ahmad, Mater H. Mahnashi, Bandar A. Alyami, Yahya S. Alqahtani, Farhat Ullah, Muhammad Ayaz, Muhammad Tariq, Abdul Sadiq*, Umer Rashid. Synthesis of Michael adducts as key building blocks for potential analgesic drugs. In-vitro, in-vivo and in-silico explorations. Drug Design, Development and Therapy. 15 (2021) 1299—1313	4.319
71.	2021	Muhammad Naeem Ahmed, Sadia Shabbir, Bakhtawar Batool, Tariq Mahmood, Umer Rashid, Khawaja Ansar Yasin, Muhammad Nawaz Tahir, M. L. Arias Cassar, Diego M. Gil. A New Insight into Non-covalent Interactions in 1,4-Disubstituted 1 H -1,2,3-Triazole: Synthesis, X-ray structure, DFT calculations, in vitro Lipoxygenase Inhibition (LOX) and in silico Studies. Journal of Molecular Structure 1236 (2021) 130283	3.841
72.	2021	Guangli Lu, Sharui Shan, Bibi Zainab, Zainab Ayaz, Jialiang He, Zhenxing Xie, Umer Rashid , Dalin Zhang, Arshad Mehmood Abbasi. Novel Vaccine Design Based on Genomics Data Analysis-A Review. Scandinavian Journal of Immunology. 2021;93:e12986	3.889 0300-9475
73.	2021	Hasnain Sajid, Sana Malik, Umer Rashid, Tariq Mahmood, Khurshid Ayub, Hydrogen adsorption on Ge52-, Ge92- and Sn92- Zintl	2.292 2210-271X




		clusters: A DFT study. Computational and Theoretical Chemistry, 2021, 1199, 113191	
74.	2021	Muhammad Bilal Tufail, Muhammad Aamir Javed, Muhammad Ikram, Mater H. Mahnashi, Bandar A. Alyami, Yahya S. Alqahtani, Abdul Sadiq, Umer Rashid. Synthesis, Pharmacological Evaluation and Molecular Modelling Studies of Pregnenolone derivatives as Inhibitors of human dihydrofolate reductase. Steroids Volume 168 (2021) 108801	2.76
75.	2021	Muhammad Alam, Ghias Uddin, Umer Rashid, Abdur Rauf*, Muslim Raza, Syed Muhammad Mukarram Shah, Syed Uzair Ali Shah ⁵ , Saima Naz ⁶ , Ajmal Khan* In vitro and in silico xanthine oxidase inhibitory potential of Benzofuran and Allopurinol isolated from <i>Viburnum grandiflorum</i> Wall. Ex DC. South African Journal of Botany, 143, 2021, 359-362	3.111
76.	2021	Maria Bibi, Naveeda Akhter Qureshi, Abdul Sadiq, Umar Farooq, Abbas Hassan, Nargis Shaheen, Irfa Asghar, Duaa Umer, Azmat Ullah, Farhan Ahmad, Muhammad Salman, Ahtaram Bibi, Umer Rashid  . Exploring the ability of dihydropyrimidine-5-carboxamide and 5-benzyl-2,4-diaminopyrimidine-based analogues for the selective inhibition of L. major Dihydrofolate reductase. European Journal of Medicinal Chemistry. 210, 2021, 112986.	7.088
77.	2021	Majid Ali, Syed Majid Bukhari*, Asma Zaidi, Farhan A. Khan, Umer Rashid, Neelum Tahir, Baseerat Rabbani, Umar Farooq. Inhibition Profiling of Urease and Carbonic Anhydrase II by High-Throughput Screening and Molecular Docking Studies of Structurally Diverse Organic Compounds. Letters in Drug Design and Discovery. Volume 18 , Issue 3 , 2021	1.099
78.	2021	Abdur Rauf, Saud Bawazeer, Umer Rashid, Mohamed A. El-Esawi, Muhammad Humayun Khan, Syed Uzair Ali Shah, Mohammad S. Mubarak, Kannan RR Rengasamy. Antiglycation and enzyme inhibitory potential of salicylalazine isolated from <i>Micromeria biflora</i> (Buch.-Ham.ex D.Don) Benth. South African Journal of Botany, Volume 143, December 2021, Pages 344-349	3.111
79.	2021	Fahad A. Alhumaydhi, Abdullah S. M. Aljohani, Umer Rashid, Zafar Ali Shah, Abdur Rauf, Naveed Muhammad, Yahya Saleh Mohamed Al-Awthan, Omar Salem Bahattab. In vivo antinociceptive, muscle relaxant, sedative and molecular docking studies of	4.132

		peshawaraquinone isolated from <i>Fernandoa adenophylla</i> (Wall. ex G. Don) Steenis. <i>ACS Omega</i> . 2021, 6, 996–1002	
80.	2021	Saud BAWAZER, Asghar KHAN, Abdur RAUF, Taibi Ben HADDA, Yahya Saleh Mohamed AL-AWTHAN, Omar Salem BAHATTAB, Umer RASHID, Inamullah KHAN, Muhammad Asif NAWAZ, Md. Sahab UDDIN, Olatunde AHMED, Mohammad Ali SHARIATI. POM Analysis and Computational Interactions of 8-Hydroxydiospyrin Inside Active Site of Protein Tyrosine Phosphatase 1B. <i>BIOCELL</i> 2021, 45(3), 751-759	1.11 0327-9545
81.	2021	Abdur Rauf, Fahad A. Alhumaydhi, Umer Rashid, Abdullah S.M. Aljohani, Yahya Saleh Mohamed Al-Awthan, Omar Salem Bahattab, Muhammad Saleem. Naphthoquinones from <i>Diospyros lotus</i> as potential urease inhibitors: In vitro and in silico studies. <i>South African Journal of Botany</i> (2020), https://doi.org/10.1016/j.sajb.2020.11.021 .	3.111
82.	2021	Naveen Kosar, Khurshid Ayub, Umer Rashid , Muhammad Imran, Naeem Ahmed, Tariq Mahmood. Electrochemical properties of halides encapsulated Na@B40 nanocages for potential applications as anodes for sodium ion batteries; A first-principles study. <i>Materials Science in Semiconductor Processing</i> . 121 (2021) 105437	4.644 1369-8001
2020			
83.	2020	Abdul Sadiq, Umer Rashid, Sadiq Ahmad, Mohammad Zahoor, Mohamed F. AlAjmi, Riaz Ullah, Omar M. Noman ⁴ , Farhat Ullah, Muhammad Ayaz, Iftikhar Khan, Zia-Ul Islam and Waqar Ali. Treating Hyperglycemia from <i>Eryngium caeruleum</i> M. Bieb: In-vitro α -glucosidase, Antioxidant, in-vivo Antidiabetic and Molecular Docking-Based Approaches. <i>Frontiers in Chemistry</i> , 2020, 8, 558641	5.545 2296-2646
84.	2020	Nisar ud Din, Niaz Ali, Zia Uddin, Nausheen Nazir, Muhammad Zahoor, Umer Rashid, Riaz Ullah, Ali S. Alqahtani, Abdulaziz M. Alqahtani, Fahd A. Naser, Mengjun Liu, Muhammad Nisar. Evaluation of cholinesterase inhibitory potential of different genotypes of <i>Ziziphus nummularia</i> , their HPLC-UV and molecular docking analysis. <i>Molecules</i> 2020, 25(21), 5011	4.927
85.	2020	Muhammad Danish, Muhammad Asam Raza, Sana Iftikhar, Muhammad Waseem Mumtaz, Muhammad N. Tahir, Umer Rashid, Khurshid Ayub. Synthesis, single-crystal X-ray diffraction, and in vitro	1.613 1434-4475

		biological evaluation of sodium, cobalt, and tin complexes of o-nitro-/o-methoxyphenylacetic acid: experimental and theoretical investigation. Monatshefte für Chemie-Chemical Monthly. 151, pages1727–1736(2020)	
86.	2020	Zafar Ali Shah, Tareq Abu-Izneid, Abdur Rauf, Umer Rashid , Maria Nizam, Naveed Muhammad, Kannan RR Rengasamy. Phosphodiesterase 1 inhibition and molecular docking study of phytochemicals isolated from stem heartwood of Heterophragma adenophyllum Seem. South African Journal of Botany 135 (2020) 274-279	3.111
87.	2020	Abida Munir, Adil Khushal, Kiran Saeed, Abdul Sadiq, Rahim Ullah, Gohar Ali, Zaman, Ashraf, Ehsan Ullah Mughal, Muhammad Saeed Jan, Umer Rashid , Izhar Hussain, Amara Mumtaz. Synthesis, in-vitro, in-vivo anti-inflammatory activities and molecular docking studies of acyl and salicylic acid hydrazide derivatives. Bioorganic Chemistry 104 (2020) 104168	5.307
88.	2020	Abdullah S.M. Aljohani, Tareq Abu-Izneid, Zafar Ali Shah, Umer Rashid, Khurshid Ayub, Abdur Rauf, Naveed Muhammad, Fahad A. Alhumaydhi, Maria Asghar, Mohammad S. Mubarak, Mohammad Ali Shariati, Haiyuan Zhang. Density Functional Theory, molecular docking and in vivo muscle relaxant, sedative, and analgesic studies of Indanone derivatives isolated from Heterophragma adenophyllum. J. Mol Str. Dynamics. 39(17):6488-6499	3.841 1538-0254
89.	2020	Muhammad Arshad; Kainat Ahmed; Zafar Iqbal; Umer Rashid; Muhammad N Arshad; Abdullah M Asiri; Tariq Mahmood. Synthesis, structural properties, enzyme inhibition and molecular docking studies of (Z)-N'-(1-allyl-2-oxoindolin-3-ylidene)methane sulfonohydrazide and (Z)-N'-(1-allyl-2-oxoindolin-3-ylidene)-3-nitrobenzenesulfonohydrazide. Molecular Structure. 221, (2020) 128880	3.841
90.	2020	Durdana Waseem, Gul Majid Khan, Ihsan-ul Haq, Umer Rashid, Deeba Nadeem Syed. The triphenyltin carboxylate derivative triphenylstannyl 2-(benzylcarbonyl)benzoate impedes prostate cancer progression via modulation of Akt/FOXO3a signaling. Toxicology and Applied Pharmacology 401 (2020) 115091.	4.46 0041-008X
91.	2020	Abdur Rauf, Tareq Abu-Izneid, Umer Rashid , Fahad Alhumaydhi, Saud Bawazeer, Anees Ahmed Khalil, Abdullah S. M. Aljohani, Emad Mohamed Abdallah, Abdel Rahman Al-Tawaha, Yahia N. Mabkhot, Mohammad ali Shariati, Sergey Plygun, Md. Sahab Uddin and Godswill Ntsomboh-Ntsefong. Anti-inflammatory, anti-bacterial, toxicological profile, and in-silico studies of dimeric	3.246





		naphthoquinones from Diospyros lotus. BioMed Research International. Volume 2020, Article ID 7942549, 10 pages	
92.	2020	Aaima Iftikhar, Muhammad Saqib Khan, Umer Rashid , Qaisar Mahmood, Habiba Zafar, Muhammad Bilal, Nadia Riaz. Influence of metallic species for efficient photocatalytic water disinfection: bactericidal mechanism of in vitro results using docking simulation. Environmental Science and Pollution Research. 27, 39819–39831(2020)	5.19 1614-7499
93.	2020	Muhammad Nadeem, Muhammad Waseem Mumtaz, Muhammad Danish, Umer Rashid , Hamid Mukhtar, Ahmad Irfan, Farooq Anwar, Nazamid Saar. UHPLC-QTOF-MS/MS Metabolites profiling and antioxidant/antidiabetic attributes of Cuscuta reflexa grown on Casearia tomentosa: Exploring phytochemicals role via molecular docking. International Journal of food Properties 2020, 23, 918–940	3.338 1532-2386
94.	2020	Muhammad Nadeem, Muhammad Waseem Mumtaz, Muhammad Danish, Umer Rashid , Hamid Mukhtar, Ahmad Irfan. Antidiabetic functionality of Vitex negundo leaves based on UHPLC-QTOF-MS/MS based bioactives profiling and molecular Docking insights.) Industrial Crops and Products 152, (2020) 112445	6.449 0926-6690
95.	2020	Muafia Jabeen Amin, Ghulam Abbas Miana, Umer Rashid , Khondaker Miraz Rahman, Hidayat-ullah Khan, Abdul Sadiq. SAR based in-vitro anticholinesterase and molecular docking studies of nitrogenous progesterone derivatives. Steroids, 158 (2020) 108599.	2.76
96.	2020	Saif Al-Hosni, Tania Shamim Rizvi, Ajmal Khan, Liaqat Ali, Najeeb Ur Rehman, Umer Rashid , Javid Hussian, Abdul Latif Khan, Ahmed Al-Harrasi. Diketopeprazin and Methyl-5-docosenoate from endophytic fungi Aureobasidium pollulan BSS6 with α -Glucosidase Inhibition and its validation through Molecular Docking. South African Journal of Botany 134 (2020) 322-328	3.111
97.	2020	Muhammad Saeed Jan; Sajjad Ahmad; Fida Hussain; Ashfaq Ahmad; Fawad Mahmood; Umer Rashid  ; Obaid-ur-Rahman Abid; Farhat Ullah; Muhammad Ayaz; Abdul Sadiq. Design, Synthesis, In-vitro, In-vivo and In-silico studies of Pyrrolidine-2,5-dione Derivatives as Multitarget Anti-inflammatory Agents. European Journal Medicinal Chemistry 186 (2020) 1118632	7.088
98.	2020	Ashfaq Ahmad, Farhat Ullah, Abdul Sadiq, Muhammad Ayaz, Haroon Rahim, Umer Rashid , Sajjad Ahmad, Muhammad Saeed Jan, Riaz Ullah, Abdelaat A. Shahat, Hafiz Majid Mahmood: Pharmacological evaluation of aldehydic-pyrrolidinedione against HCT-116, MDA-MB231, NIH/3T3, MCF-7 cancer cell lines, antioxidant and enzyme	4.319





		inhibition studies. Drug Design, Development and Therapy, 13 (2019) 4185–4194.	
99.	2020	Muhammad Umar Farooq, Muhammad Waseem Mumtaz, Hamid Mukhtar, Umer Rashid , Muhammad Tayyab Akhtar, Syed Ali Raza, Muhammad Nadeem. UHPLC-QTOF-MS/MS based phytochemical characterization and anti-hyperglycemic prospective of hydro-ethanolic leaf extract of Butea monosperma. Nature Scientific Reports 10 (2020) 3530	4.996 2045-2322
2019			
100.	2019	Gulraiz Ahmad, Nasir Rasool, Komal Rizwan, Imran Imran, Ameer Zahoor, Muhammad Zubair, Abdul Sadiq, Umer Rashid  , Synthesis, In-Vitro Cholinesterase Inhibition, In-Vivo Anticonvulsant Activity and In-Silico Exploration of N-(4-Methylpyridin-2-yl)thiophene-2-carboxamide Analogs. Bioorganic Chemistry 92 (2019) 103216	5.307
101.	2019	Fida Hussain, Zeeshan Khan, Muhammad Saeed Jan, Sajjad Ahmad, Ashfaq, Ahmad, Umer Rashid  , Farhat Ullah, Muhammad Ayaz, Abdul Sadiq. Synthesis, in-vitro α -glucosidase inhibition, antioxidant, in-vivo antidiabetic and molecular docking studies of pyrrolidine-2,5-dione and thiazolidine-2,4-dione derivatives. Bioorganic Chemistry Volume 91 (2019) 103128	5.307
102.	2019	Muhammad Taha, Noor Barak Almandil, Umer Rashid, Muhammad Ali, Mohamed Ibrahim, Mohammed Gollapalli, Ashik Mosaddik, Khalid Mohammed Khan. 2,5-Disubstituted Thiadiazoles as Potent β -glucuronidase Inhibitors; Synthesis, In Vitro and In Silico Studies. Bioorganic Chemistry, 91 (2019) 103126	5.307
103.	2019	Muhammad Nadeem · Muhammad Waseem Mumtaz · Muhammad Danish · Umer Rashid · Hamid Mukhtar, Farooq Anwar · Syed Ali Raza. Calotropis procera: UHPLC-QTOF-MS/MS based profiling of bioactives, antioxidant and anti-diabetic potential of leaf extracts and an insight into molecular docking. Journal of Food Measurement and Characterization, 13 (4) (2019) 3206–3220.	3.006 2193-4134
104.	2019	Muhammad Saeed Jan, Muhammad Shahid, Sajjad Ahmad, Fida Hussain, Ashfaq Ahmad, Fawad Mahmood, Umer Rashid, Farhat Ullah, Nadir Zaman Khan, Muhammad Aasim, Muhammad Ayaz, Jehangir Khan, Abdullah, Abdul Sadiq, Synthesis of Pyrrolidine-2,5-dione Based Anti-inflammatory drug: In-vitro COX-2, 5-LOX Inhibition and In-vivo Anti-inflammatory Studies, Latin American Journal of Pharmacy 38 (11): 2287-94 (2019)	0.229 2362-3853

105.	2019	Saba Tahir; Tariq Mahmood; Faiqa Dastgir; Ihsan ul-Haq; Amir Waseem; Umer Rashid  . Design, Synthesis and Anti-bacterial Studies of Piperazine Derivatives against Drug Resistant Bacteria. Eur. J. Med. Chem 166 (2019) 224-231	7.088
106.	2019	Saba Tahir Tanoli, Muhammad Ramzan, Abbas Hassan, Abdul Sadiq, Muhammad Saeed Jan, Farhan A. Khan, Farhat Ullah, Haseen Ahmad, Maria Bibi, Tariq Mahmood, Umer Rashid  . Design, Synthesis and Bioevaluation of Tricyclic Fused Ring System as Dual Binding Site Acetylcholinesterase Inhibitors. Bioorganic Chemistry 83 (2019) 336–347	5.307
107.	2019	Umar Farooq; Sadia Naz; Afshan Shams; Yasir Raza; Ayaz Ahmed; Umer Rashid  ; Abdul Sadiq. <i>Isolation of dihydrobenzofuran derivatives from ethnomedicinal species Polygonum barbatumas anticancer compounds. Biological Research 52 (2019) 1</i>	7.634 0717-6287
108.	2019	Niaz Muhammad, Naseer Ali Shah, Saqib Ali, Sadaf Noor Elahi, Wajid Rehman, Shaukat Shujah, Muhammad Rashid Khan, Abdul Wadood, Mehreen Ghufraan, Umer Rashid. Theoretical and experimental in vitro antifungal and antitumor activities of organotin(IV) derivatives of 3-(4-nitrophenyl)-2-methylacrylic acid. Pharmaceutical Chemistry Journal Vol. 53, No. 8, 2019, 689-696	1.069 0091-150X
109.	2019	Muhammad Arshad, Muhammad Waseem Mumtaz, Ayoub Rashid Chaudhary, Umer Rashid, Mukhtar Ali, Hamid Mukhtar, Ahmad Adnan and Syed Ali Raza. Metabolite profiling of Cycas revoluta leaf extract and docking studies on alpha-glucosidase inhibitory molecular targets by phytochemicals. Pak. J. Pharm. Sci., Vol.32, No.2(Suppl), March 2019, pp.871-874	0.863
2018			
110.	2018	Muhammad Danish, Muhammad Asam Raza, Uzma Anwar, Umer Rashid and Zaheer Ahmed. Differential Functional Theory and Molecular Docking Studies of Newly Synthesized Carbamates. J Chin Chem Soc. (Accepted)	1.967
111.	2018	Muhammad Sarfraz, Umer Rashid, Nargis Sultana, Muhammad Ilyas Tariq. Synthesis, x-rays analysis, docking study and cholinesterase inhibition activity of 2,3-dihydroquinazolin-4(1H)-one derivatives. Iranian Journal of Chemistry and Chemical Engineering (IJCCE)	1.903

112.	2018	Mumtaz Ali, Sardar Ali, Momin Khan, <u>Umer Rashid</u> , Manzoor Ahmad, Ajmal Khan, Ahmed Sulaiman Al-Harrasi, Farhat Ullah, Abdul Latif. Synthesis, biological activities, and molecular docking studies of 2-mercaptobenzimidazole based derivatives. Bioorganic Chemistry 80 (2018) 472-479	5.307
113.	2018	Yousaf Ali, Shafida Abd Hamid, <u>Umer Rashid</u> . Biomedical Applications of Aromatic Azo Compounds: From Chromophore to Pharmacophore. Mini Reviews in Med. Chem. DOI : 10.2174/1389557518666180524113111.	3.737
114.	2018	Muhammad Taha, <u>Umer Rashid</u> , Syahrul Imran, Muhammad Ali. Rational design of bis-indolylmethane-oxadiazole hybrids as inhibitors of Thymidine phosphorylase. Bioorg. Med. Chem. 26 (2018) 3654-3663.	3.461
115.	2018	Fatima Iftikhar, Farhana Yoqoob, Nida Tabassum, Muhammad Saeed Jan, Abdul Sadiq, Saba Tahir, Tahira Batool, Basit Niaz, Farzana Latif Ansari, Muhammad Iqbal Chaudhary and <u>Umer Rashid</u>  . Design, Synthesis, In-Vitro Thymidine Phosphorylase Inhibition, In-Vivo Antiangiogenic and In-Silico Studies of C-6 substituted dihydropyrimidines. Bioorganic Chemistry 80 (2018) 99–111	5.307
116.	2018	Anwar Zeb, Farhat Ullah, Sajjad Ahmad, Muhammad Ayaz, <u>Umer Rashid</u> and Abdul Sadiq. Chemical characterization, analgesic, antioxidant and anticholinesterase potentials of essential oils from <i>Isodon rugosus</i> Wall. ex. Benth. Front. Pharmacol. – Ethnopharmacology 2018; 9: 623.	5.988
117.	2018	Muafia Jabeen, Muhammad Iqbal Choudhry, Ghulam Abbas Miana, Khondaker Miraz Rahman, <u>Umer Rashid</u> , Hidayat-ullah Khan, Arshia and Abdul Sadiq. Synthesis, Pharmacological Evaluation and Docking Studies of Progesterone and Testosterone Derivatives as Anticancer Agents. Steroids 136 (2018) 22-31	2.76
118.	2018	Naeem Akhtar Virk, Aziz-ur-Rehman, Muhammad Athar Abbasi, Sabahat Zahra Siddiqui, <u>Umer Rashid</u> , Javed Iqbal, Muhammad Saleem, Muhammad Ashraf, Wardah Shahid, Syed Adnan Ali Shah. Conventional versus microwave assisted synthesis, molecular docking and enzyme inhibitory activities of new 3,4,5-trisubstituted-1,2,4-triazole analogues. Pakistan Journal of	0.863

		Pharmaceutical Sciences Vol.31, No.4(Suppl), July 2018, pp.1501-1510	
119.	2018	Murtaza Madni, Muhammad Naeem Ahmed, Shahid Hameed, Syed Wadood Ali Shah, Umer Rashid , Khurshid Ayub, M. Nawaz Tahir, Tariq Mahmood. Synthesis, quantum chemical, in vitro acetyl cholinesterase inhibition and molecular docking studies of four new coumarin based pyrazolylthiazole nuclei. J Mol. Structure Volume 1168 (2018) 175-186	3.841
120.	2018	Muafia Jabeen, Sajjad Ahmad, Khadija Shahid, Abdul Sadiq, Umer Rashid  . Ursolic Acid Hydrazide Based Organometallic Complexes: Synthesis, Characterization, Antibacterial, Antioxidant and Docking Studies. Front. Chem. 6 (2018) 1-14	5.545
121.	2018	Atta Ullah, Fatima Iftikhar, Muhammad Arfan, Syeda Tayyaba Batool Kazmi, Muhammad Naveed Anjum, Ihsan-ul Haq, Muhammad Ayaz, Sadia Farooq, Umer Rashid  . Amino Acid Conjugated Antimicrobial Drugs: Synthesis, Lipophilicity- Activity Relationship, Antibacterial and Urease Inhibition Activity. European Journal of Medicinal Chemistry 145 (2018) 140-153	7.088
122.	2018	Muhammad Naeem Ahmed, Khawaja Ansar Yasin, Sadiq-ur-Rehman, Rashid Mehmood, Umer Rashid , Tariq Mahmood, Khurshid Ayub, Muhammad Nawaz Tahir and Abdul Majeed Khan, Synthesis, Characterization, Anti-leishmanial Activity and in silico Studies of 5-(4-methoxyphenyl)-2-(undecylthio)-1,3,4-oxadiazole, Journal of the Chemical Society of Pakistan (2018) (Accepted)	0.698
2017			
123.	2017	Fawad Mahmood, Muhammad Saeed Jan, Sajjad Ahmad, Umer Rashid , Muhammad Ayaz, Farhat Ullah, Fida Hussain, Ashfaq Ahmad, Arif-ullah Khan, Muhammad Aasim, Abdul Sadiq. Ethyl 3-oxo-2-(2,5-dioxopyrrolidin-3-yl)butanoate derivatives: Anthelmintic and cytotoxic potentials, antimicrobial and docking studies. Front. Chem 2017; 5: 119.	5.545
124.	2017	Huzaifa Hanif, Samina Nazir, Kehkashan Mazhar, Muhammad Waseem, Shazia Bano, Umer Rashid  . Targeted delivery of	

		mesoporous silica nanoparticles loaded Monastrol into cancer cells: An in vitro study. Applied Nanoscience 2017, 7, 549–555.	3.869
125.	2017	Fatima Iftikhar, Yousaf Ali, Farooq Ahmad Kiani, Syed Fahad Hassan, Tabeer Fatima, Ajmal Khan, Basit Niaz, Abbas Hassan, Farzana Latif Ansari and Umer Rashid  . Design, Synthesis, In Vitro Evaluation and Docking studies on Dihydropyrimidine-Based Urease Inhibitors. Bioorganic Chemistry. 2017, 74, 53-65.	5.307
126.	2017	Mumtaz Ali, Sultan Muhammad, Raza Shah, Ajmal Khan, Umer Rashid , Umar Farooq, Farhatullah, Abdul Sadiq, Muhammad Ayaz, Majid Ali, Manzoor Ahmad, Abdul Latif, Neurologically Potent Molecules from Crataegus oxyantha; Isolation, Anticholinesterase Inhibition and Molecular Docking . Front. Pharmacol. 8 (327) (2017) 1-11.	5.988
127.	2017	Nargis Sultana, Muhammad Sarfraz, Saba Tahir Tanoli, Muhammad Safwan Akram, Abdul Sadiq, Umer Rashid  , Muhammad Ilyas Tariq. Synthesis, Crystal structure determination, biological screening and docking studies of N1-substituted derivatives of 2,3-dihydroquinazolin-4(1H)-one as inhibitors of cholinesterases . Bioorganic Chemistry. 72 (2017) 256–267.	5.307
128.	2017	Muhammad Taha, Nor Hadiani Ismail, Muhammad Ali, Umer Rashid , Syarul Imran, Nizam Uddin, Khalid Mohammed Khan. Molecular hybridization conceded exceptionally potent quinolinyloxadiazole hybrids through phenyl linked thiosemicarbazide antileishmanial scaffolds: In silico validation and SAR studies . Bioorganic Chemistry 71 (2017) 192-200.	5.307
129.	2017	Hamid Nawaz, Amir Waseem, Zia-ur-Rehman, Muhammad Nafees, Muhammad Nadeem Arshad, Umer Rashid  . Synthesis, characterization, cytotoxicity and computational studies of new phosphine and carbodithioate based palladium(II) complexes . Applied Organometallic Chemistry, 31 (11) (2017) 3771	4.072
130.	2017	Muhammad Sarfraz, Nargis Sultana, Umer Rashid  , Muhammad Safwan Akram, Abdul Sadiq, Muhammad Ilyas Tariq, Synthesis, biological evaluation and docking studies of 2,3-dihydroquinazolin-4(1H)-one derivatives as inhibitors of cholinesterases Bioorganic Chemistry 70 (2017) 237–244	5.307
131.	2017	Huma Fatima, Naveeda Akhter Qureshi*, Nargis Shaheen, Umer Rashid, Muhammad Fiaz Qamar. In vivo antiplasmodial potential	

		of aqueous extracts of trachyspermum ammi and punica granatum seeds in male balb/c mice. Acta Poloniae Pharmaceutica- Drug Research Vol. 74 No. 6 pp. 1781ñ1795, 2017	0.555
2016			
132.	2016	Umer Rashid  , Waqas Ahmad, Syed Fahad Hassan, Naveeda Akhtar Qureshi, Basit Niaz, Bakhtiar Muhammad, Sameera Imdad, Muhammad Sajid. <i>Design, synthesis, antibacterial activity and docking study of some new trimethoprim derivatives.</i> (2016) Bioorganic and Medicinal Chemistry Letter. 26 (2016) 5749–5753.	2.94
133.	2016	Sufyan Ahmad, Fatima Iftikhar, Farhat Ullah, Abdul Sadiq, Umer Rashid  <i>Rational design and synthesis of dihydropyrimidine based dual binding site acetylcholinesterase inhibitors.</i> Bioorganic Chemistry 69 (2016) 91-101.	5.307
134.	2016	Wajid Rehman, Rehana Yasmeen, Fazal Rahim, Muhammad Waseem, Cun-Yue Guo, Zonera Hassan, Umer Rashid  and Khurshid Ayub. <i>Synthesis biological screening and molecular docking studies of some tin (IV) Schiff base adducts.</i> Journal of Photochemistry & Photobiology, B: Biology. 164 (2016) 65-72.	6.814
135.	2016	Naveeda Akhtar Qureshi, Abid Ali, Umer Rashid, Tayyab-ur-Rehman and Naeem Ali. <i>Prevalence of Leishmania tropica in School Boys of Khyber Agency, FATA near Pak-Afghan Border.</i> Acta Tropica 164 (2016) 90-94.	3.222
136.	2016	Abdul Wadood, Mehreen Ghufraan, Syed Fahad Hassan, Huma Khan, Syed Sikandar Azam, Umer Rashid  ; <i>In silico identification of promiscuous scaffolds as potential inhibitors of 1-deoxy-D-xylulose 5-phosphate reductoisomerase for treatment of falciparum malaria.</i> Pharmaceutical Biology 55 (2017) 19-32	3.889
137.	2016	Umer Rashid, Fazal Rahim, Muhammad Taha, Muhammad Arshad, Hayat Ullah, Tariq Mahmood, Muhammad Ali. Synthesis of 2-Acylated and Sulfonated 4-hydroxycoumarins: In vitro Urease Inhibition and Molecular Docking Studies. Bioorganic Chemistry 66 (2016) 111-116	5.307

138.	2016	Umer Rashid  , Riffat Sultana, Nargis Shaheen, Syed Fahad Hassan, Farhana Yaqoob, Muhammad Jawad Ahmad, Fatima Iftikhar, Nighat Sultana, Saba Asghar, Masoom Yasinzai, Farzana Latif Ansari, Naveeda Akhter Qureshi. Structure based medicinal chemistry-driven strategy to design substituted dihydropyrimidines as potential antileishmanial agents. <i>European Journal of Medicinal Chemistry</i> 115 (2016) 230-244	7.088
139.	2016	Fazal Rahim, Shifaullah, Muhammad Ali, Hayat Ullah, Umer Rashid , Muhammad Taha, Wajid Rehman, Muhammad Tariq Javed,. Synthesis and molecular docking study of bis thiobarbiturate derivatives as effective inhibitors of urease. <i>Chinese Chemical Letters</i> 27 (2016) 693-697.	8.455
140.	2016	Muhammad Jawad Ahmad, Syed Fahad Hassan, Riffat Un Nisa, Khurshid Ayub, Muhammad Shahid Nadeem, Samina Nazir, Farzana Latif Ansari, Naveeda Akhter Qureshi and Umer Rashid  . Synthesis, in vitro potential and computational studies on 2-amino-1,4-dihydropyrimidines as multitarget antibacterial ligands. <i>Med. Chem. Res.</i> 25 (2016) 1877-1894.	2.351
2015			
141.	2015	Syed Majid Bukhari, Iftikhar Ali, Asma Zaidi, Naseem Iqbal, Tayyaba Noor, Rashad Mehmood, Muhammad Salman Chishti, Basit Niaz, Umer Rashid , Muhammad Atif; Pharmacology and synthesis of Daurichromenic acid as a potent anti-HIV agent. <i>Acta Poloniae Pharmaceutica- Drug Research, Vol. 72 (6) (2015) 1059-1071.</i>	0.555
142.	2015	Umer Rashid  , Syed Fahad Hassan, Samina Nazir, Abdul Wadood, Farzana Latif Ansari, Synthesis, docking studies, and in silico ADMET predictions of some new derivatives of pyrimidine as potential KSP inhibitors. <i>Med. Chem. Res.</i> 24 (2015) 304-315	2.351
2014			
143.	2014	Samina Nazir, Tajammul Hussain, Umer Rashid , Alexander MacRobert, Nanomaterials in combating cancer: Therapeutic	

		applications and developments, Nanomedicine: Nanotechnology, biology and medicine, 10 (2014) 19-34	6.454
144.	2014	Wajid Rehman, Sirajul Haq ¹ , Bakhtiar Muhammad, Fahad Hassan, Amin Badshah, Muhammad Waseem, Fazal Rahim, Obaid-ur-Rahman Abid, Farzana Latif Ansari and Umer Rashid ✓ Organotin (IV) based complexes as promiscuous antibacterials: Synthesis, in vitro, in silico pharmacokinetic and docking studies, J of Organometallic Chemistry. 767 (2014) 91-100.	2.345
145.	2014	Saba Noor; Muhammad Waseem; Umer Rashid; Wajid Rehman, Fabrication and Some Physical Features of NiO Coated SiO₂ and SiO₂ Coated NiO. Chin. Chem. Lett. 25 (2014) 819–822	8.455
146.	2014	Muhammad Waseem, Sajida Munsif, Umer Rashid , Imad-ud-Din, Physical properties of α-Fe₂O₃ nanoparticles fabricated by modified hydrolysis technique, Applied Nanoscience, 4 (2014) 643-648	3.869
147.	2014	Muhammad Irshad, Syed Mustafa, Muhammad Waseem, Khizar Hussain Shah and Umer Rashid, Effect of temperature and electrolyte concentration on the surface charge properties of Fe(OH) ₃ . J. Chem. Soc. Pak. 36 (2014) 783-787.	0.698
2013			
148.	2013	Syed Fahad Hassan, Umer Rashid ✓, Farzana Latif Ansari, Zaheer-ul-Haq. Bioisosteric approach in designing new monastrol derivatives: An investigation on their ADMET prediction using in silico derived parameters. J. Mol. Graphics Modell. 45 (2013) 202-210	2.942
149.	2013	Umer Rashid , Iram Batool, Abdul Wadood, Ajmal Khan, Zaheer-ul-Qasmi, Iqbal Chaudary and Farzana Latif Ansari. Structure based virtual screening-driven identification of monastrol as a potent urease inhibitor” J. Mol. Graphics Modell. 43 (2013) 47-57	2.942
150.	2013	Saima Kalsoom, Umer Rashid , M. Ahmad Mesaik, Omer Mohamed Abdalla, Khalida Hussain, Waqasuddin Khan, Awais Shaukat, Fatima Iftikhar, Muhammad Baseer Khan, Zaheer-ul-Haq and Farzana Latif Ansari, In vitro and in silico exploration of	2.351

		<i>IL-2 inhibition of small organic molecules. Med Chem Res</i> 22 (2013) 5739-5751	
151.	2013	Umer Rashid, Ahsanullah, Muhammad Waseem, Farzana Latif Ansari, <i>Microwave assisted partial synthesis of enantiomerically pure S-ispinesib-A case study, J. Chem. Soc. Pak.</i> 35 (2013) 846-858.	0.698
152.	2013	Wajid Rehman, Zonera Hassan, Umer Rashid, Fazal Rahim, Obaid-Ur-Rahman Abid, <i>Synthesis, Characterization Antibacterial and Antifungal activity of some transition metal complexes, Med. Chem. Res.</i> 23 (2014) 2207–2211	2.351
153.	2014	Muhammad Waseem, S. Mustafa, A. Naeem, K.H. Shah, Umer Rashid, <i>Synthesis, physical characteristics, and Cd²⁺ sorption studies of amorphous Fe(OH)₃, Desalination and Water Treatment</i> , 52 (2014) 4783–4791	1.273
154.	2013	Syed Mustafa, Muhammad Irshad, Muhammad Waseem, Khizar Hussain Shah, Umer Rashid and Wajid Rehman, <i>Adsorption of heavy metal ions in ternary systems onto Fe(OH)₃. Korean J. Chem. Eng.</i> 30(12) (2013), 2235-2240	3.146
2008			
155.	2008	Farzana Latif Ansari, Fatima Iftikhar, Ihsan-ul-Haq , Bushra Mirza, Mohammad Baseer, Umer Rashid, <i>Solid-phase synthesis and biological evaluation of a parallel library of 2,3-dihydro-1,5-Benzothiazepines. Bioorg. Med. Chem.</i> 2008, 16, 7691–7697.	3.461