
CURRICULUM VITAE

(Impact Factor: 418.542)

Personal data:

Family Name, First Name : Ejaz, Syeda Abida

Place of Birth : Bahawalpur, Punjab, Pakistan

Postal Address in Pakistan : House No. B-III 2521, Mohallah Mubarak
Pura, Bahawalpur, Pakistan
Department of pharmaceutical Chemistry,
Khawaja Fareed Campus, The Islamia
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Objectives : To acquire a challenging position in a progressive and dynamic organization where the organizational culture emphasizes continuous learning, team work, creativity, trust and respect for each other and opportunities for exploiting knowledge and experience.

Academic Career/Degrees held:

1st Degree : Ph.D

Main Subject : Pharmaceutical Chemistry

Host University : COMSATS University Islamabad-Abbottabad Campus, Pakistan

Title of Thesis : **Identification and Characterization of Pharmacological Inhibitors of Alkaline Phosphatase Isozymes & Nucleotide Pyrophosphatases**

Duration of Studies : September, 2013- April , 2018 (4 years)

Degree Result : GPA 3.56/4.00

Supervisor : Prof. Dr. Jamshed Iqbal

2nd Degree : M.Phil

Main Subject : Pharmaceutical Chemistry

University : The Islamia University of Bahawalpur, Pakistan

Duration of Studies : 2011-2013 (Two Years)

Degree Result : 565.0/680 (83.09%)

3rd Degree : Pharm-D

Main Subject : Pharmaceutical Chemistry, Pharmaceutics & Pharmacology

University : The Islamia University of Bahawalpur, Pakistan

Duration of Studies : 2005-2010 (Five Years)

Degree Result : 2986/4550 (66.6 %)

4th Degree : Intermediate

Main Subject : Pre-Medical

BISE : Bahawalpur, Punjab , Pakistan

Duration of Studies : 2003-2005 (Two Years)

Degree Result : 800/1100 (72.27 %)

5th Degree : SSC

BISE : Bahawalpur, Punjab , Pakistan

Duration of Studies : 2000-2002 (Two Years)

Degree Result : 688/850

Research Skills:

High-throughput Screening Assays and cancer cell line expertise	<ul style="list-style-type: none">• Have an excellent experience for 7 years of enzyme inhibition studies; recombinant, extracted as well as commercial enzymes.• Have an excellent experience for 4 years with cancer cell line (BHK-21, HeLa (cervical Cancer cells), MCF-7 (Breast Cancer cells), MDA-MB-231 (Breast Cancer cells), K-562 (Lymphoblast) and MC3T3 (Pre-osteoblast cells) handling and their functional assays.
Others/ Expertise in instruments	<ul style="list-style-type: none">• Cytotoxicity assays including: MTT assay, SRB assay and Caspase Activity• Cell cycle analysis and Apoptosis assays• DNA binding Assays• Flow Cytometry, capillary electrophoresis and Fluorescence Microscopy• PCR and RT-PCR, western blot, Gel Doc• Antioxidant Assays, Antibacterial & Antifungal Assays, Malachite Green Assay• Enzyme Inhibition and Kinetic Studies of Enzymes including: Acetyl and Butyryl Cholinesterases, Lipoxygenase, Chymotrypsin, Tyrosinase, α-glucosidase, β-glucosidase, Aldose reductase, Alkaline phosphatase, Nucleotidase pyrophosphatase, Ecto-5-nucleotidase, nucleoside triphosphate diphosphohydrolases, Carbonic anhydrase, Monoamine oxidase Lipase.• Homology Modelling and Molecular docking studies• DFTs studies, QSAR studies• Phytochemical analysis, Total phenolic and total flavonoid contents assay

International Visits

1. Three months (Aug.-Oct. 2015) research training at Department of Pharmacy, University of Bonn, Germany under DAAD funded project "International Master of Science in Drug Research".
2. Three months (Aug.-Oct. 2014) research training at Department of Pharmacy, University of Bonn, Germany under DAAD frame project "Cooperation between German and Pakistani Universities".
3. Two weeks study tour to German Universities (Gottingen, TU Berlin, Bonn, Saarland, and various Pharma industries on DAAD summer project from 03/03/2014 to 13/03/2014.

Service experience (Teaching/Professional Experience)

1. Currently Working as Assistant Professor of Pharmaceutical Chemistry (31st Jan, 2020-todate) in the Department of Pharmacy, The Islamia University of Bahawalpur.
2. Worked as an Assistant Professor of Pharmaceutical Chemistry (18th April,2018-25th Jan-2020) in the Department of Pharmacy, Women Institute of Learning Science, Abbottabad, Pakistan
3. Worked as Community Pharmacist (1st April 2011 to 30th April, 2013) at host Pharma Medical Store, Bahawalpur, Pakistan

Supervision of research students:

- Supervised 08 MS Students

Sr. No.	Student Name	Topics	Current Status
1	Mubashir Aziz	A Comprehensive Computational Approach for the Identification of Potent Inhibitors of NEK7: A Novel Target for Anti-Cancer Drug Discovery	completed
2	Amna Saeed	An Extensive Computational Approaches Towards Aldo-keto reductases (AKRs) as Attractive Targets for Anticancer Drug Discovery and Development	completed
3	Hafiz Mohammad Kashif Mahmood	Identification and Characterization of Heterocyclic Compounds as Potential Inhibitors of Cholinesterase and Monoamine Oxidases Isozymes using QSAR and In-silico Structural Modifications	Completed

4	Muhammad Sajjad Bilal	Identification of pharmacological Inhibitors of Epidermal Growth Factor Receptor and Vascular Endothelial Growth Factor Receptors Via Computer Aided Drug Design	Completed
5	Ammara Fayyaz	In silico approaches for the Identification of Coumarins as Potential Neuroprotective Agents for the Treatment of Alzheimer's disease by Targeting Cholinesterases and Monoamine Oxidases	Completed
6	Hafiz Muhammad Attaullah	Newly Synthesized Azo-Thiohydantoin and Adamantyl Derivatives as Potential Alkaline Phosphatase Inhibitors: Evidence from Biochemical Characterizations, Molecular Modelling and Pharmacokinetics Studies	Research in progress
7	Junaid Abbasi	Research in progress	
8	Romaisa	Research In progress	

➤ Supervised 04 PhD Students

Sr. No.	Student Name	Topics	Current Status
1	Mubashir Aziz	Never in mitosis gene A- related kinases as a Novel target of anti-cancer drugs discovery: Pharmacophore Based Virtual Screening, Synthesis, Characterization, Biochemical Evaluation & Computational Studies	Synopsis Approved
2	Aftab Ahmed	Synthesis, In vitro Evaluation and Computational Investigations of Selective Inhibitors of Human Ecto-nucleotidases: Potential Role in Type 2 Diabetes	Synopsis Approved
3	Muhammad Sajjad Bilal	Synthesis and Biochemical Characterization of Iminothiazolidine and Sulphonamide Derivatives as the Potential Inhibitor of Dickkopf1 (Dkk-1) Protein: A Novel Target for the Treatment of Different Cancers	Synopsis Approved
4	Ammara Fayyaz	Synopsis Approval in progress	

Participation in Conferences / Workshops

- A virtual Event: Collaboration Among OIC Members Countries for Promotion of Research Culture in Medicines and Vaccines Through Strengthening and Upgrading the Clinical Trials. June 3rd, 2021, Organized by COMSTech Secretariat, Islamabad, Pakistan.
- An Advanced Training Course on "How to Establish Halal Products Testing Laboratory?", 8-10 June, 2021, Organized by COMSTech Secretariat, Islamabad, Pakistan.
- Lab Safety Training, Jan 12th, 2021, Organized by Office of Occupational Safety and Health, The Islamia University of Bahawalpur.
- STEMS International Conference, March 30-31, 2021, Organized by Directorate of International Linkages, The Islamia University of Bahawalpur.
- Breast Cancer Awareness & Screening Program (BCASSP-2021). October 26th, 2021, Organized by Medical Division, The Islamia University of Bahawalpur.

Research Projects (in progress)

- ***"Computational and Biochemical Analysis of Heterocyclic Compounds against Emerging Targeted Enzymes: Anticancer Drug Development"***. An ORIC IUB funded Research Project.

References:

1. Prof. Dr. Amara Mumtaz, Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad, Pakistan. Email: amaramumtaz@cuiatd.edu.pk
2. Dr Pervaiz Ali channar, Department of chemistry, Dawood university, Karachi, Pakistan.. Email: pervaiz.ali@duet.edu.pk
3. Dr.Farhan Siddique, Department of Pharmacy, Bahauddin University, multan, Pakistan. . Email: drfarhansiddique@bzu.edu.pk

List of Publications

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2025

1. Laamari Y, Fawzi M, **Syeda Abida Ejaz**, Aziz M, Ali O, Alotaibi SH, Alossaimi MA, Dehbi O, Riadi Y, Auhmani A. Exploration of new thiazolidinones derived from natural verbenone: Design, synthesis, characterization, and in silico evaluation of alkaline phosphatase and carbonic anhydrase-II inhibition activity. *Journal of Molecular Structure*. 2025 Feb 15;1322:140332.
2. Shakir SA, Rashid U, Fatima N, **Syeda Abida Ejaz**, Fayyaz A, Ullah MZ, Saeed A, Khan A, Al Harrasi A, Mumtaz A. Exploration of novel triazolo-thiadiazine hybrids of deferasirox as multi-target-directed anti-neuroinflammatory agents with structure–activity relationship (SAR): a new treatment opportunity for Alzheimer's disease. *RSC advances*. 2025;15(1):101-18.
3. Riadi Y, Geesi MH, **Syeda Abida Ejaz**, Afzal O, Oubella A. Design, characterization, and DFT exploration of new quinazoline-N-substituted analogs: Anti-cancer activity and molecular docking insights. *Journal of Molecular Structure*. 2025 Feb 15;1322:140420.

2024

4. M. Aziz, **Syeda Abida Ejaz**, P.A. Channar, A. G. Alkhatami, T. Qadri, Z. Hussain, M. Hussain & R. Ujan. Identification of dimethyl 2,2'-((methylenebis(2-(2H-benzo[d][1,2,3]triazol-2-yl)-4-(2,4,4-trimethylpentan-2-yl)-6,1phenylene))bis(oxy))diacetate (TAJ4) as antagonist of NEK-Family: a future for potential drug discovery. *BMC Cancer* 2024, 24, 1521-1543. **(ISI-indexed Q2 Journal, Impact Factor 4.095)**.
5. Bimoussa, A., Mourad, F., Oubella, A., Alossaimi, M.A., Riadi, Y., **Syeda Abida Ejaz**, Aziz, M., Fayyaz, A., Auhmani, A. and Itto, M.Y.A., 2024. Multitargeted molecular docking and dynamics simulation studies of thiazolidinones synthesised from (R)-carvone against specific tumour protein markers: Synthesis, spectroscopic characterization and in-silico study. *Journal of Molecular Structure*, 1318, p.139171. **(ISI-indexed Q2 Journal, Impact Factor 4.095)**.
6. Ullah MZ, Hussain Z, Shakir SA, Mahmood M, **Syeda Abida Ejaz**, Aziz M, Fayyaz A, Iqbal J, Mumtaz A. Exploration of newly synthesized deferasirox derivatives as potential anti-cancer agents via in-vitro and in-silico approaches. *International Journal of Biological Macromolecules*. 2024 Dec 1;283:137971. **(ISI-indexed Q2 Journal, Impact Factor 4.095)**.
7. Haider MB, Saeed A, Azeem M, Ullah SA, **Syeda Abida Ejaz**, Attaullah HM. Putting forward novel sulfonamide-thiazole-pyrazoline hybrids as potential central core structure for the development of non-specific b-TNAP and c-IAP inhibitors. *International journal of*

biological macromolecules. 2024 Dec;283(Pt 3):137699. (**ISI-indexed Q2 Journal, Impact Factor 4.095**).

8. Ali H, Jabeen Q, Jamshed A, **Syeda Abida Ejaz**, Qadeer M, Anwaar M, Rasheed HM. Evaluation of Antiurolithiatic Effects of *Moringa oleifera* Lam. Leaves Extract: In-vitro, in-silico and in-vivo Approaches. Dose-Response. 2024 Nov 12;22(4):15593258241301222. (**ISI-indexed Q2 Journal, Impact Factor 4.095**).
9. Bimoussa A, Oubella A, Alossaimi MA, Aziz M, Attaullah HM, **Syeda Abida Ejaz**, Morjani H, Auhmani A, Robert A, Riahi A, Riadi Y. Novel Bis-1, 2, 3-triazole-thiazolidinone hybrid as anticancer agents that induce apoptosis and molecular modeling study. *Future Medicinal Chemistry*. 2024 Nov 1;16(21):2193-210. (**ISI-indexed Q2 Journal, Impact Factor 4.095**).
10. Alshehri MM, Alshammari MK, Alghazwani MK, **Syeda Abida Ejaz**, Aziz M, Alshehri AM, Alanazi RH, Alshlali OM, Mahzari AM, Alharbi BH, Sarfraz M. In silico study of some plant compounds as potential anticancer agents targeting MALT1 allosteric domain. *Journal of Biomolecular Structure and Dynamics*. 2024 Sep 20:1-6. (**ISI-indexed Q2 Journal, Impact Factor 4.095**).
11. Nawaz Z, Riaz N, Saleem M, Iqbal A, **Syeda Abida Ejaz**, Muzaffar S, Bashir B, Ashraf M, Rehman AU, Bilal MS, Prabhala BK. Probing N-substituted 4-(5-mercapto-4-ethyl-4H-1, 2, 4-triazol-3-yl)-N-phenylpiperidine-1-carboxamides as potent 15-LOX inhibitors supported with ADME, DFT calculations and molecular docking studies. *Heliyon*. 2024 Sep 15;10(17).
12. **Syeda Abida Ejaz**, Alsfook AA, Shamim T, Sumreen L, Mahmood HK, Li C. Identification of Quinolone-Triazole Hybrids As Potential Inhibitors Using In Silico Approach. *Química Nova*. 2024 Aug 2;48(2):e-20250032.
13. Anjum F, Touqeer S, Khan MY, Jamil Q, Rida A, Shirazi JH, **Syeda Abida Ejaz**, Attaullah HM, Sarwar G, Khan ZH, Wazir MA. Pharmacognostic Evaluation, Chemical Characterization, and Antibacterial Activity of *Bassia indica* (Wight) AJ Scott. *Plants*. 2024 Jun 25;13(13):1753.
14. Siddique F, Daoui O, Ayoub M, Elkhatabi S, Chtita S, Afzal S, Mohyuddin A, Kaukab I, **Syeda Abida Ejaz**, Salamatullah AM, Ibenmoussa S. Identification and in silico screening of natural phloroglucinols as potential PI3K α inhibitors: A computational approach for drug discovery. *Open Chemistry*. 2024 Jul 19;22(1):20240064.
15. H. M. Attaullah, **Syeda Abida Ejaz***, P. A. Channar, A. Saeed, R. Ujan, S. Zargar, S. A. Channar, R. Sahito, T. A Wani, Q. Abbas. Exploration of newly synthesized azothiohydantoin as the potential alkaline phosphatase inhibitors via advanced biochemical characterization and molecular modeling approaches. *BMC chemistry*. 2024, 18(1): 1-15. (**ISI-indexed Q2 Journal, Impact Factor 4.095**).
16. Ahmed A, Channar PA, Ejaz SA, Saeed A, Saleem M, Shamim T, Wani TA, Hussain J, Gul N, Khan S, Zargar S. Synthesis of small size adamantane-linked aminothiazoles as potent inhibitors of urease, α -glucosidase and carbonic anhydrase and their molecular docking studies. *Chemical Papers*. 2024 Jun 21:1-24.

17. A. Manan, H. Z. Tariq, **Syeda Abida Ejaz***, A. Saeed, A. Ahmed, A. Ahmed, T. A Wani, M. Saleem, J. Hussain, G. Shabir, H. El-Seedi. N-Adamantanyl-2-(2-(phenyl) hydrazone)-3-oxobutanamides endowed with dual inhibitors of urease and α -glucosidase: Design, synthesis, and computational studies. Results in Chemistry. 2024, 101399. (**ISI-indexed Q3 Journal, Impact Factor 2.31**).
18. S. Jalil, R. Basri, M. Aziz, Z. Shafiq, **Syeda Abida Ejaz**, A. Hameed, J. Iqbal. Pristine 2-chloroquinoline-based-thiosemicarbazones as multitarget agents against alzheimer's disease: In vitro and in silico studies of monoamine oxidase (MAO) and cholinesterase (ChE) inhibitors. Journal of Molecular Structure. 2024, 1306(15) 13784. (**ISI-indexed Q3 Journal, Impact Factor 3.841**).
19. **Syeda Abida Ejaz***, B. A. Khan, P. A. Channar, M. Aziz, E. U. Mughal, A. Saeed, L. Sumreen, Z. Hussain, M. Hussain, R. Ujan, M. Elhadi, A. Sadiq, T. Hökelek. DABCO-PEG ionic liquid catalyzed synthesis, single-crystal structure, and antioxidant activity of a flavanone derivative. AIP Advances. 2024, 14, 025133. (**ISI-indexed Q3 Journal, Impact Factor 1.697**).
20. Z. Nawaz, N. Riaz, M. Saleem, A. Iqbal, **Syeda Abida Ejaz**, B. Bashir, S. Muzaffar, M. Ashraf, M. S. Bilal, B. K. Prabhala, S. Sajid. Molecular hybrids of substituted phenylcarbamoylpiperidine and 1, 2, 4-triazole methylacetamide as potent 15-LOX inhibitors: Design, synthesis, DFT calculations and molecular docking studies. Bioorganic Chemistry. 2024, 143, 106984. (**ISI-indexed Q1 Journal, Impact Factor 5.307**).
21. M. Sarfraz, M. K. Ibrahim, **Syeda Abida Ejaz***, H. M. Attaullah, M. Aziz, M. Arafat, T. Shamim, M. Elhadi, T. Ruby, H. K. Mahmood. An Integrated Computational Approaches for Designing of Potential Piperidine based Inhibitors of Alzheimer Disease by Targeting Cholinesterase and Monoamine Oxidases Isoenzymes. Applied Biochemistry and Biotechnology. 2024 Volume 196, pages 5875–5902. (**ISI-indexed Q3 Journal, Impact Factor 3.094**).
22. **Syeda Abida Ejaz***, M. Sarfraz, M. Aziz, T. A Wani, T. Ruby, S. Zargar, M. Arafat, C. Li. Evaluation of Cytotoxic Activity and Apoptosis-Inducing Potential of 5, 6, 7-Trihydroxyflavone against Breast Cancer and Cervical Cancer Cell Lines. Journal of biological regulators and homeostatic agents. 2024, 38(1): 303-317. (**ISI-indexed Q3 Journal, Impact Factor 2.843**).

2023

23. M. N. Mustafa, P. A. Channar, M. Sarfraz, A. Saeed, **Syeda Abida Ejaz***, M. Aziz, F. A. Alasmay, H. Y. Alsoqair, H. Raza, S. J. Kim, A. Hamad. Synthesis, kinetic studies and in-silico investigations of novel quinolinyl-iminothiazolines as alkaline phosphatase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry. 38 (2023): 2163394. (**ISI-indexed Q1 Journal, Impact Factor 5.758**).
24. A. Ahmed, A. Ahmed, P. A. Channar, **Syeda Abida Ejaz***, A. A Alsouk, A. Saeed, R. Ujan, Q. Abbas, T. Hökelek, M. Bolte. Synthesis, single crystal XRD, in-silico and in-vitro studies of alkyl substituted acyl thiourea as carbonic anhydrase inhibitor. Journal of Molecular

Structure. 1292 (2023): 136187. **(ISI-indexed Q3 Journal, Impact Factor 3.841)**

25. M. Aziz, **Syeda Abida Ejaz***, N. Tamam, F. Siddique. A comprehensive computational approach for the identification of structure-based potential pharmacological candidates as selective AKR1B1 and AKR1B10 inhibitors: repurposing of purine alkaloids for the treatment of cancer. *Journal of Biomolecular Structure and Dynamics*, 2023, 41 (16): 7892-7912. **(ISI-indexed Q1 Journal, Impact Factor 5.235)**.
26. S. Alrokayan, T. Hussain, S. Alamery, A. A. Mohammed, A. Mahmood, **Syeda Abida Ejaz**, P. Langer, J. Iqbal. [1, 8]-Naphthyridine derivatives as dual inhibitor of alkaline phosphatase and carbonic anhydrase. *BMC Chemistry*, 2023, 17(1): 142. **(ISI-indexed Q2 Journal, Impact Factor 4.095)**.
27. M. Aziz, **Syeda Abida Ejaz***, B. A Alsouk, A. Sultan, C. Li. Identification of potential inhibitors against E. coli via novel approaches based on deep learning and quantum mechanics-based atomistic investigations. *Archives of Biochemistry and Biophysics*. 2023, 747: 109761. **(ISI-indexed Q2 Journal, Impact Factor 4.114)**.
28. M. Aziz, **Syeda Abida Ejaz***, H. M. Rehman, A. SA Alsubaie, KH. Mahmoud, F.Siddique, MS Al-Buriah, ZA Alrowaili. Identification of NEK7 inhibitors: Structure based virtual screening, molecular docking, density functional theory calculations and molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, 2023, 41(14): 6894-6908. **(ISI-indexed Q1 Journal, Impact Factor 5.235)**.
29. **Syeda Abida Ejaz***, A. Farid, S. Zargar, P. A. Channar, M. Aziz, T. A Wani, H. M. Attaullah, R. Ujhan, A. Tehzeeb, A. Saeed, H. S. Ali, M. F Erben. Computational and theoretical chemistry of newly synthesized and characterized 2,2'-(5,5'-(1,4-phenylene)bis(1H-tetrazole-5,1-diyl))bis-N-acetamides. *BMC Chemistry*, 2023, 17(1): 97. **(ISI-indexed Q3 Journal, Impact Factor 2.31)**.
30. **Syeda Abida Ejaz***, M. Aziz, A. Fayyaz, T. A Wani, S. Zargar. Computer-aided approach for the identification of lead molecules as the inhibitors of cholinesterase's and monoamine oxidases: novel target for the treatment of Alzheimer's disease. *Journal of the Serbian Chemical Society*, 2023 (89) 2, Pages: 177-194. **(ISI-indexed Q4 Journal, Impact Factor 1.11)**.
31. M. N. Mustafa, P. A. Channar, **Syeda Abida Ejaz***, S. Afzal, M. Aziz, T. Shamim, A. Saeed, A. A Alsouk, R. Ujan, Q. Abbas, T. Hökelek. Synthesis, DFT and molecular docking of novel (Z)-4-bromo-N-(4-butyl-3 (quinolin-3-yl)thiazol-2(3H)-ylidene)benzamide as elastase inhibitor. *BMC Chemistry*. 2023, 17(1): 95. **(ISI-indexed Q3 Journal, Impact Factor 2.31)**.
32. **Syeda Abida Ejaz***, M. Aziz, T. A Wani, H. M Al-Kahtani. Evaluation of mechanical features and antibacterial potential of fluoroquinolone against β -ketoacyl-ACP synthases (FabB, FabF & FabH) via computational approaches. *Archives of Biochemistry and Biophysics*, 2023, 744: 109674. **(ISI-indexed Q2 Journal, Impact Factor 4.114)**.
33. M. Yasin, W. Shahid, M. Ashraf, M. Saleem, S. Muzaffar, A.-ur-Rehman, **Syeda Abida Ejaz**, H. M. K. Mahmood, K. Bhattarai, N. Riaz. Targeting new N-furfurylated 4-chlorophenyl-

1,2,4-triazolepropionamide hybrids as potential 15-lipoxygenase inhibitors supported with in vitro and in silico studies. *Journal of Biomolecular Structure and Dynamics*, 2023, 44(11): 5166-5182. (ISI-indexed Q1 Journal, Impact Factor 5.235).

34. **Syeda Abida Ejaz***, M. Z.-ul-Abideen, P. A. Channar, A. Saeed, A. Ahmed, N. S. Alsaiari, K. M. Katubi, Q. Abbas, K. A Dahlous, H. Raza, S. J. Kim, M. N. Mustafa. Synthesis, biochemical characterization and molecular modeling studies of 5-(substituted benzylidene) pyrimidine-2, 4, 6-trione: Potential inhibitors of alkaline phosphatase. *Journal of Molecular Structure*. 2023, 1282: 135225. (ISI-indexed Q3 Journal, Impact Factor 3.841)
35. P. A. Mahesar, P. A. Channar, **Syeda Abida Ejaz***, A. Saeed, F.F. Alharbi, T. Shamim, M. Aziz, R. Ujan, G. A. Kandhro, S. A. Channar, Q. Abbas, M. Hussain. Potential role of hydrazinyl 1, 2, 4-triazoles derivatives as acetylcholinesterase inhibitors: synthesis, biological evaluation, kinetics mechanism and molecular docking and simulation studies. *Chemical Papers*, 2023, 77(6): 3447-3459. (ISI-indexed Q3 Journal, Impact Factor 2.146).
36. **Syeda Abida Ejaz***, M. Aziz, M. F. Ramadan, A. Fayyaz, M. S. Bilal. Pharmacophore-Based Virtual Screening and In-Silico Explorations of Biomolecules (Curcumin Derivatives) of *Curcuma longa* as Potential Lead Inhibitors of ERBB and VEGFR-2 for the Treatment of Colorectal Cancer. *Molecules*, 2023, 28 (10): 4044. (ISI-indexed Q1 Journal, Impact Factor 4.6).
37. A. Saeed, S. Ashraf, M. Aziz, P. A. Channar, **Syeda Abida Ejaz***, A. Fayyaz, Q. Abbas, F. A. Alasmay, A. M. Karami, A. Tehzeeb, A. Mumtaz, H. R El-Seedi. Design, synthesis, biochemical and in silico characterization of novel naphthalene-thiourea conjugates as potential and selective inhibitors of alkaline phosphatase. *Medicinal Chemistry Research*, 2023. (ISI-indexed Q4 Journal, Impact Factor 2.351).
38. N.Riaz, M. Yasin, M. Ashraf, M. Saleem, B. Bashir, A. Iqbal, **Syeda Abida Ejaz**, S. Ejaz, H. M. K. Mahmood, K. Bhattarai. Vetting of new N-furfurylated p-chlorophenyl-1,2,4-triazole acetamides as lipoxygenase inhibitors assisted with in vitro and in silico studies. *Journal of the Iranian Chemical Society*, 2023, 20 (4): 977-994. (ISI-indexed Q3 Journal, Impact Factor 2.271).
39. **Syeda Abida Ejaz***, A. A Alsfook, G. El-S. Batiha, A. T. Aborode, S. R. Ejaz, H. I. Umar, M. Aziz, A. Saeed, H. M. K. Mahmood, A. Fayyaz. Identification of N-(4-acetyl-4, 5-dihydro-5-(7, 8, 9-substituted-tetrazolo [1, 5-a]-quinolin-4-yl)-1, 3, 4-thiadiazol-2-yl) acetamide derivatives as potential caspase-3 inhibitors via detailed computational investigations. *Structural Chemistry*, 2023, 34(2), 425-438. (ISI-indexed Q4 Journal, Impact Factor 1.014).
40. **Syeda Abida Ejaz***, M. Aziz, Z. Zafar, N. Akhtar, H. A Ogaly. Revisiting the inhibitory potential of protein kinase inhibitors against NEK7 protein via comprehensive computational investigations. *Scientific Reports*, 2023, 13(1):4304. (ISI-indexed Q2 Journal, Impact Factor 4.996).
41. B. Bashir, N. Riaz, **Syeda Abida Ejaz***, M. Saleem, A. Iqbal, M. Ashraf, S. Ejaz, A.-ur -Rehman, M. Aziz, K. Bhattarai. Investigations of p-tolyloxy-1, 3, 4-oxadiazole propionamides as soybean 15-lipoxygenase inhibitors in comforting with in vitro and in silico studies. *Journal*

of Biomolecular Structure and Dynamics, 2023, 1-20. (ISI-indexed Q1 Journal, Impact Factor 5.235).

42. B. Bashir, N. Riaz, **Syeda Abida Ejaz***, M. Saleem, A. Iqbal, H. M. K. Mahmood, S. Ejaz, M. Ashraf, K. Bhattarai. Parsing p-tolyloxy-1, 3, 4-oxadiazolepropanamides as 15-lipoxygenase inhibitors prop up by in vitro and in silico profiling including structure determination. Journal of Molecular Structure. 2023, 1275: 134664. (ISI-indexed Q3 Journal, Impact Factor 3.841)
43. **Syeda Abida Ejaz***, M. Aziz, A. Ahmed, S. S Alotaibi, S. M Albogami, F. Siddique, G. El-S. Batiha. New Insight into the pharmacological importance of atropine as the potential inhibitor of AKR1B1 via detailed computational investigations: DFTs, ADMET, molecular docking, and molecular dynamics studies, Applied Biochemistry and Biotechnology, 2023. (ISI-indexed Q3 Journal, Impact Factor 3.094).
44. A. Saeed, H. Z. Tariq, G. Shabir, T. Hökelek, M. Bolte, **Syeda Abida Ejaz***, A. Ahmed. Green synthesis, X-ray crystallography, DFT and Hirshfeld analysis of C-2 symmetric 1, 3-bis (4-ethylphenyl) triaz-1-ene. Journal of Molecular Structure, 2023, 1274, 134523. (ISI-indexed Q3 Journal, Impact Factor 3.841)
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