Dr. YOUSAF KHAN



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Google Scholar https://scholar.google.com/citations?user=K34iVAkAAAAJ&hl=en

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"Exceptionally energetic and enthusiastic person...projects a charisma that captures the imagination of peoples...demonstrated excellent classroom and lab management skill..."

"Committed to do work in an organization where I can utilize my abilities and skills with great passions…."

Personal information:

Father Name: **Nadir Khan**
Address: Department of Chemistry, COMSATS university Islamabad (45550), Islamabad.
CNIC# 56503-3135940-9
Date of Birth 25/12/1985

Professional Profile:

Eager to bring the students into the twenty-first century using a unique combination of education experience coupled with computer background in systems management.

- Hold Ph.D. degree in Organic Chemistry
- Expert in organic Synthesis and computational studies.
- Experienced in use of the Internet and educational software.
- Dedicated to enthusiastic and dynamic teaching as a means of creating and nurturing a lifelong love of knowledge in students.
- Currently working as Lecturer BPS-17 in Higher & Technical Education, Government of Baluchistan, Pakistan.

Education, Honors and Certifications:

- **Gold Medal in MS-Chemistry (2018)**

SSC	(2000)	**Science**	BBISE Quetta Baluchitan
F.Sc	(2002)	**Pre-Medical**	BBISE Quetta Baluchitan
B.Sc	(2005)	**Zoo. Chem. Geo**	University of Baluchistan, Quetta, Baluchistan
M.Sc	(2007)	**Organic Chemistry**	Quaid-e-Azam University, Islamabad
M.S	(2018)	**Organic Chemistry**	BUITEMS Quetta, Baluchistan
Ph.D	(2024)	**Organic Chemistry**	COMSATS University Islamabad, Islamabad

Professional Qualifications:

B.Ed	(2015)	**Science**	University of Baluchistan, Quetta, Baluchistan
M.Ed	(2019)	**Science**	Al-Hamd Islamic University, Quetta, Baluchistan

Ph.D Research Title:

Transformation of Simple Organic Molecules into Bio-active Five-membered Heterocyclic Scaffolds and their Enzyme Inhibition Study

Department of Chemsitry

COMSATS University, Islamabad, Pakistan, (FA20- PCH-001)

Supervisor: **Dr. Aneela Maalik**

Email: aneela.maalik@comsats.edu.pk

M.S. Research Title:

Synthesis and biological evaluation of aliphatic Schiff base as a promising drug candidate

Impact Factor

270+

GOOGLE SCHOLAR

https://scholar.google.com/citations?user=K34iVAkAAAAJ&hl=en

Cited by

	All	Since 2020
Citations	1187	1176
h-index	21	21
i10-index	37	37

List of Publications:

Books Chapter & Review Article

1. **Yousaf Khan,** Maalik, A., Hashmi, M.Z., Farooq, U., Nawaz, M., Rehman, Z.U., Sattar, A. and Ahmad, B., **2022**. Endocrine-disrupting compounds. In Environmental Micropollutants (pp. 183-199). **Elsevier**.
2. **Yousaf Khan,** Maalik, A., Hakimullah, Sattar, A., Mazhar, D., Hashmi, M.Z., Bibi, M., Aslam, S., Ullah, S.A. and Ahmed, B., **2024.** Current Trends in the Development of Vaccines from Micro to Industrial Level. In Recent Advances in Industrial Biochemistry (pp. 371-397). Cham: ***Springer International Publishing***.
3. **Yousaf Khan**, Mukhtiar, A., Arooj, K., Rehman, A., Khan, S., & Panizai, Z. U. R. (2025). Structural Properties of Lignin. In Handbook of Lignin (pp. 1-33). Singapore: **Springer Nature** Singapore.
4. **Yousaf Khan**, Sattar, A., Ullah, S. A., Rehman, W., Khan, S., Hussain, R., & Gulshan, U. (2025). Rice Husk Based Bio-composites. In Rice Husk Biomass: Processing, Properties and Applications (pp. 235-270). Singapore: **Springer Nature** Singapore.
5. **Yousaf Khan**, Sattar, A., Ullah, S.A., Bibi, M., Sarfraz, H. and Mukhtiar, A., 2024. Chemicals That Disrupt the Endocrine System and Their Effects on Behavior. Kashmir Journal of Science, 3(2).

Research Publication

1. **Yousaf Khan**, Maalik, A., Rehman, W., Sarfraz, H., Hussain, R., Khan, S., & Adnan, R. (2025). Facile 3-chloro-1H-indazole based 1, 3, 4-thiadiazole derivatives as novel thymidine phosphorylase and anti-diabetic inhibitors: Experimental, in-vitro and molecular modelling approaches. **Naunyn-Schmiedeberg's Archives of Pharmacology**, 1-19.
2. **Yousaf Khan**, Aneela Maalik, Wajid Rehman, Mohammed M Alanazi, Shoaib Khan, Rafaqat Hussain, Liaqat Rasheed, Abdul Saboor & Shahid Iqbal, Synthesis, in vitro bio-evaluation and in silico molecular docking studies of thiadiazole-based Schiff base derivatives; **Future medicinal Chemistry**, 2024, 16(4), 0276.
3. **Yousaf Khan**, Sarfraz, H., Rehman, W., Khan, M., Rasheed, L., & Rahman, K. U. (2025). Innovative Horizons in Drug Design: Exploring the Synthesis and Medicinal Properties of Heterocyclic Schiff Bases. A Review. **Mini-Reviews in Medicinal Chemistry**, 25(10), 727-744.

4. **Yousaf Khan,** Hussain, R., Rehman, W., Khan, S., Maalik, A., Iqbal, T., Aziz, T., Afridi, M.I., Alharbi, M. and Alasmari, A.F., 2024. In-vitro and in-silico assessment of thiazole-thiazolidinone derivatives as selective inhibitors of urease and α-glucosidase. **Future Medicinal Chemistry**, pp.1-10.

5. **Yousaf Khan,** Shahid Iqbal*, Mazloom Shah, Aneela Maalik, Rafaqat Hussain, Shoaib Khan*, Imran Khan et al. "New quinoline-based triazole hybrid analogs as effective inhibitors of α-amylase and α-glucosidase: Preparation, in vitro evaluation, and molecular docking along with in silico studies." ***Frontiers in chemistry*** 10 (2022).

6. **Yousaf Khan,** Wajid Rehman, Rafaqat Hussain, Shoaib Khan, Aneela Malik, Marwa Khan, Anjum Liaqat et al. "New biologically potent benzimidazole-based-triazole derivatives as acetylcholinesterase and butyrylcholinesterase inhibitors along with molecular docking study." ***Journal of Heterocyclic Chemistry*** (2022).
7. **Yousaf Khan,** Maalik, A., Rehman, W., Rafaqat Hussain, Shoaib Khan, Alanazi, M.M., Asiri, H.H. and Iqbal, S., 2023. Identification of Novel Oxadiazole-Based Benzothiazole Derivatives as Potent Inhibitors of α-Glucosidase and Urease: Synthesis, In Vitro Bio- Dr Rafaqat Hussain Page 7 of 8 evaluation and Their In Silico Molecular Docking Study. ***Journal of Saudi Chemical Society,*** p.101682.

8. **Yousaf Khan,** Shoaib Khan*****, Wajid Rehman, Rafaqat Hussain, Aneela Maalik, Farhan Ali, Muhammad Usman Khan, Abdul Sattar, and Mohammed A. Assiri. "Hybrid Molecules of Thiadiazole-Based Benzothioate and Benzenesulfonothioate: Synthesis, Structural Analysis, and Evaluation as Potential Inhibitors of Thymidine Phosphorylase and β-Glucuronidase through In Vitro and In Silico Approaches." ***Journal of Molecular Structure*** (2023): 136439.

9. **Yousaf Khan,** Wajid Rehman, Rafaqat Hussain, Shoaib Khan, and Aneela Maalik. "Benzothiazole-Based 1, 3, 4-Thiadiazole Hybrids Derivatives as Effective Inhibitors of Urease and Thymidine phosphorylase: Synthesis, In Vitro and In Silico Approaches." ***Journal of Molecular Structure*** (2023): 135945.

10. **Yousaf Khan,** Shoaib Khan, Rafaqat Hussain, Aneela Malik, Wajid Rehman, Mohamed W.Attwa, Rafia Masood, Hany W. Darwish, Hazem A. Ghabbour. "The Synthesis, In Vitro Bio-Evaluation, and In Silico Molecular Docking Studies of Pyrazoline- Thiazole Hybrid Analogues as Promising Anti-α-Glucosidase and Anti-Urease Agents." **Pharmaceuticals** (2023):161650

11. **Yousaf Khan**, Shoaib Khan, Rafaqat Hussain, Wajid Rehman, Aneela Maalik, Urooba Gulshan, Mohamed A. Attwa, Hamy W. Darwish, Hazem A. Ghabbou, Nawab Ali. "Identification of Indazole-Thiadiazole bearing Thiazolidinone Hybrid Derivatives:Theoretical and Computational Approaches to develop promising Anti-Alzheimer's Candidates." **Pharmaceuticals** (2023) 2717503.

12. **Yousaf Khan**, Mukhtiar, A., Sarfraz, H., Khan, S., Hussain, R., Naeem, M. U., ... & Jabbir, F. (2025). Unveiling of the novel benzothiazole derived thiazolidinone derivatives: in vitro and in silico insights to design a promising agent for anti-Alzheimer's disease. **Zeitschrift für Naturforschung C**, (0), 1-10.

13. **Yousaf Khan**, Hussain, R., Rehman, W., Khan, S., Maalik, A., Iqbal, T., & Alasmari, A. F. (2024). In-vitro and in-silico assessment of thiazole-thiazolidinone derivatives as selective inhibitors of urease and α-glucosidase. **Future Medicinal Chemistry**, 16(24), 2627-2636.

14. **Yousaf Khan**, Khan, S., Hussain, R., Mukhtar, A., Sarfraz, H., & Aminullah, S. (2025). Medicinal approaches toward diabetes mellitus based on chloro-1 H-indazole-derived triazolo-thiadiazole hybrid derivatives: design, synthesis, characterization, in vitro and in silico insights. **Journal of the Iranian Chemical Society**, 1-19.

15. Amjid, Z., Khan, S., Iqbal, T., Hussain, R., Ali, H.Z., Shoaib, K., **Yousaf Khan***, Ullah, H., Arshad, S., Iqbal, R. and Ullah, R., 2024. Synthesis, confirmations and biological evaluation of acid substituted Schiff base derivatives: unraveling insight through SAR, DFT, ADMET and molecular docking**. Results in Chemistry**, 11, 101744.

16. Farghaly, T. A., Rehman, W., **Yousaf Khan**, & Sarfraz, H. (2025). Synthesis, biological screening and computational analysis of Thiazole linked Thiazolidinone Schiff bases as anti-Alzheimer's drug candidates. Bioorganic Chemistry, 108812.

17. Baqi, A., Samiullah, Khan, J., Sadiq, A., **Yousaf Khan**, Ali, S., & Bourhia, M. (2025). Computational identification and experimental validation of novel Saccharum officinarum microRNAs along with their targets through RT-PCR approach. Plant Signaling & Behavior, 20(1), 2452334.

18. Baqi, A., Samiullah, Rehman, W., Bibi, I., Menaa, F., **Yousaf Khan,** Albalawi, D.A. and Sattar, A., 2023. Identification and Validation of Functional miRNAs and Their Main Targets in Sorghum bicolor. **Molecular Biotechnology,** pp.1-15.

19. Shoaib Khan, Rehman, W., Rahim, F., Hussain, R., Obaidullah, A.J., Alotaibi, H.F., Alanazi, M.M., Khan, M.U. and **Yousaf Khan, 2023**. Bis-indole based triazine derivatives: Synthesis, characterization, in vitro β-glucuronidase anti-cancer and anti-bacterial evaluation along with in silico molecular docking and ADME analysis. ***Arabian Journal of Chemistry***, *16*(8), p.104970.

20. Shoaib Khan, Hayat Ullah, Fazal Rahim, Rafaqat Hussain, **Yousaf Khan,** Muhammad Saleem Khan, Rashid Iqbal, Baber Ali, and Mohammed Fahad Albeshr. "Synthesis, biological evaluation and molecular docking study of pyrimidine based thiazolidinone derivatives as potential anti-urease and anti-cancer agents." ***Journal of Saudi Chemical Society*** (2023): 101688.

21. Shoaib, Khan*, Rafaqat Hussain, **Yousaf Khan,** Tayyiaba Iqbal, Hany W. Darwish, and Mohamed GH Ali. "Novel bis-thiazole-thiazolidinone hybrid derivatives: Synthesis, structural properties and anticholinesterase bioactive potential as drug competitor based on docking studies." ***Journal of Molecular Structure*** 1303 (2024): 137417.

22. Shoaib Khan, Rafaqat Hussain, **Yousaf Khan,** Tayyiaba Iqbal, Tariq Aziz, Metab Alharbi. “Correlation between In Vitro Anti-Urease Activity and In Silico Molecular Modelling Approach of Novel Imidazopyridine-Oxadiazole Hybrids Derivatives.” **Open Chemistry** (2024)

23. Hussain, Rafaqat, Shoaib Khan*, **Yousaf Khan,** Tayyiaba Iqbal, Saeed Anwar, Tariq Aziz, and Metab Alharbi. "Development of promising acetylcholinesterase and butyrylcholinesterase inhibitors: Synthesis, in vitro and in silico approaches of pyridine derived fused bis-oxadiazole and bis-thiadiazole derivatives." ***Journal of Molecular Structure*** (2024): 138228.

24. Shoaib Khan*, Rafaqat Hussain, **Yousaf Khan,** Tayyiaba Iqbal, Saeed Anwar, Tariq Aziz, Metab Alharbi. “In vitro enzymatic, in silico ADME and molecular docking based analysis for identification of novel bis-indole containing triazine-thiazole hybrids derivatives as promising urease inhibitors”. ***Zeitschrift für Naturforschung C*** (2024)

25. Rafaqat Hussain*, Shoaib Khan*, **Yousaf Khan,** Tayyiaba Iqbal. “A promising

acetylcholinesterase and butyrylcholinesterase inhibitors: In vitro enzymatic and in silico molecular docking studies of benzothiazole-based oxadiazole containing imidazopyridine hybrid derivatives". ***Result in Chemistry*** (2024):101503

26. Khan, S., Ullah, H., Hussain, R., Khan, M.U., **Yousaf Khan**, Hussain, A., Iqbal, T., Ali, H., Iqbal, R., Akram, M.I. and Almutairi, S.M., 2024. Design, synthesis, in vitro biological assessment and in silico molecular modeling study of thiazole-thiazolidinone derivatives as potent anti-cancer agents. **Results in Chemistry**, 101507.

27. Shoaib Khan, Rafaqat Hussain, Tayyiaba Iqbal, **Yousaf Khan**, Urooj Jamal, Hany W. Darwish, Muhammad Adnan. "Identification of novel benzothiazole-thiadiazole-based thiazolidinone derivative: In vitro and in silico approaches to develop promising anti-Alzheimer's agents". ***Future Medicinal Chemistry*** (2024).

28. Shoaib Khan, Rafaqat Hussain, **Yousaf Khan,** Tayyiaba Iqbal, Muhammad Bilal Khan, Khairia Mohammed Al-Ahmary 4, Saedah R. Al Mhyawi. "Insight into role of triazole derived Schiff base bearing sulfonamide derivatives in targeting Alzheimer's disease: Synthesis, characterization, in vitro and in silico assessment". ***Journal of Molecular Structure*** (2024): 138845.

29. Shoaib Khan, Rafaqat Hussain, **Yousaf Khan,** Tayyiaba Iqbal, Farman Ullah, Shifa Felemban, M.M. Khowdiary. "Facile benzothiazole-triazole based thiazole derivatives as novel thymidine phosphorylase and α-glucosidase inhibitors: Experimental and computational approaches". ***Enzyme and Microbial Technology*** (2024): 110470

30. Shoaib Khan*, Rafaqat Hussain, **Yousaf Khan**,Tayyiaba Iqbal, Khurram Shoaib and Uzma Jehangir, M.M. Khowdiary Shifa Felemban. "Developing Correlation Between In Silico Molecular Modeling and In Vitro α Amylase, Anti-Cancer and SARS-COV-2 Studies of Bis-Indole Derived Triazine-Based Thiazolidinone Hybrid Derivatives". ***ChemistrySelect*** (2024): e202400686

31. Shoaib Khan, Rafaqat Hussain, Hayat Ullah, **Yousaf Khan**, Tayyiaba Iqbal, Saeed Anwar. "Identification of 1,2,4-Triazole-Bearing Bis Schiff Base Hybrid Scaffold: In Vitro and In Silico Insights to Develop Promising Anti-Urease, Anti-Cancer Agents." ***Results in Chemistry*** **(2024):** 101540

32. Shoaib Khan, **Yousaf Khan**, Ayman M. Al-Qaaneh, Rafaqat Hussain, Tayyiaba Iqbal, Hayat Ullah, Khurram Shoaib et al. "Exploring effective diagnosis of Alzheimer disease: Experimental and computational analysis of hybrid benzimidazole based thiazolidinone derivatives." ***Results in Chemistry*** 9 (2024): 101663.

33. Shoaib Khan, Rafaqat Hussain, **Yousaf Khan**, Tayyiaba Iqbal, Saeed Anwar, Tariq Aziz, Muhammad Irfan Afridi, Metab Alharbi, and Fayez Alghamdi. "Investigation of pyridine-bearing thiazolidinone derivatives as promising inhibitors of thymidine phosphorylase and α-glucosidase: Theoretical and computational approaches to develop multitarget drugs." ***Journal of Molecular Structure*** 1319 (2025): 139324.

34. Shoaib Khan, Tayyiaba Iqbal, **Yousaf Khan**, Rafaqat Hussain, Muhammad Saleem Khan, Hayat Ullah, Tayyaba Zahoor et al. "Experimental and computational pharmacological approaches decoding the anti-diabetic molecular mechanism of indole based triazole bearing sulfonothioate derivatives." ***Results in Chemistry*** (2024): 101707.

35. Khan, Shoaib, Rafaqat Hussain, **Yousaf Khan**, Tayyiaba Iqbal, Saeed Anwar, Tariq Aziz, Muhammad Irfan Afridi, Metab Alharbi, and Fayez Alghamdi. "Investigation of pyridine-bearing thiazolidinone derivatives as promising inhibitors of thymidine phosphorylase and α-glucosidase: Theoretical and computational approaches to develop multitarget drugs." ***Journal of Molecular Structure*** 1319 (2025): 139324.

36. Maalik, A., Khan, I., Rehman, W., Faiz, S., Alanazi, A.S., Hefnawy, M., Rasheed, L., Hassan, S.I., Hussain, R., Abdellattif, M.H., Shakeel, M., **Yousaf Khan,** 2025. Discovery of thiourea based acetylcholinesterase inhibitors and antibacterial agents: Synthesis, in vitro, structure-activity relationship and in silico study. Journal of Molecular Structure, 1321, 140082.

37. Khan, S., Hussain, R., **Yousaf Khan,** Iqbal, T., Anwar, S., Aziz, T. and Alharbi, M., 2024. In silico DFT and molecular modeling of novel pyrazine-bearing thiazolidinone hybrids derivatives: elucidating in vitro anti-cancer and urease inhibitors. Zeitschrift für Naturforschung C, (0).

38. Khan, S., Hussain, R., **Yousaf Khan,** Iqbal, T., Islam, M.S. and Almutairi, T.M., 2024. Synthesis, confirmation based on in vitro and in silico study of thiadiazole-based thiazolidinone scaffolds: An approach toward Covid-19. Results in Chemistry, 12, p.101845.

39. Iqbal, T., Khan, S., Hussain, R., **Yousaf Khan**, Rahim, F., Hayat, A., Awwad, N.S. and Alkhathami, A.G., 2025. A versatile inhibitory approach and molecular mechanism on cancer cells and cholinesterase enzymes: Synthesis, DFT, ADMET and molecular docking of thiadiazole and oxadiazole derivatives. Journal of Molecular Structure, 1322, p.140325.

40. Khan, S., Iqbal, T., Hussain, R., **Yousaf Khan,** Fiaz, Z., Rahim, F. and Darwish, H.W., 2024. Synthesis, Characterizations, Anti-Diabetic and Molecular Modeling Approaches of Hybrid Indole-Oxadiazole Linked Thiazolidinone Derivatives. Pharmaceuticals, 17(11), p.1428

41. Hawsawi, M., Khan, S., Iqbal, T., Hussain, R., **Yousaf Khan,** Zahoor, T. and Dera, A.A., 2024. Synthesis, characterization and molecular modeling approach of hybrid pyrazole based thiazolidinone derivatives: An estimation and inhibition of diabetes mellitus. Journal of Molecular Structure, 140407.

42. Khan, S., Iqbal, T., Khan, M.B., Hussain, R., **Yousaf Khan**, and Darwish, H.W., 2024. Novel pyrrole based triazole moiety as therapeutic hybrid: synthesis, characterization and anti-Alzheimer potential with molecular mechanism of protein ligand profile. BMC chemistry, 18(1), p.223.

43. Iqbal, T., Khan, S., Hussain, R., **Yousaf Khan**, Shoaib, K., Rozeena, Saeed, M. and Darwish, H.W., 2024. Novel indole based fused triazole-thiadiazole derivatives as anti-diabetic agents: in vitro and in silico approaches. Future Medicinal Chemistry, 16(23), pp.2475-2486.

44. Hussain, R., Afridi, M.I., Khan, S., **Yousaf Khan**, Iqbal, T., Rasheed, L., Islam, M.S. and Dahlous, K.A., 2025. Insight from molecular modeling and ADMET analysis: Design, synthesis and in vitro acetylcholinesterase and butyrylcholinesterase assessment of thiazolidinone containing benzoxazole hybrids derivatives. Journal of Molecular Structure, 1322, p.140589.

Key Qualifications:

Experience in teaching and computer skills and having full commands on pharmaceutical applications.

Plan and instruct each subject area using wide variety of teaching aids, motivational and implementation strategies to engage students in active learning.

Computer Skills:

Software Guess View, Autodock tools, DSV, MOE, SwissDoc, Pymol, ChimeraX, Microsoft Windows ® and Microsoft Word, PageMaker, front page, Books in Print, Microsoft excel, Microsoft PowerPoint, Microsoft access, Adope, Ulead etc

Expertise:

Strong hold on Organic Synthesis and Drug Designing.

Expert in Molecular docking studies, DFT and ADMET Predictions.

Expert in running Lab instruments and reaction strategies

Languages:

English, Urdu, Pashto.