



Dr. Saimah Khan is an Associate Professor at Integral University with over 15 years of teaching and research experience in environmental chemistry and wastewater treatment. She has an extensive publication record, including 28 research papers, 5 books, and 12 book chapters, and has presented more than 26 research papers at national and international conferences. Her research expertise encompasses constructed wetlands, pharmaceutical wastewater treatment, microplastics, air quality assessment, and sustainable water treatment technologies. She has successfully completed three research projects and is currently serving as Co-Principal Investigator on three ongoing collaborative research projects with King Khalid University, Saudi Arabia.



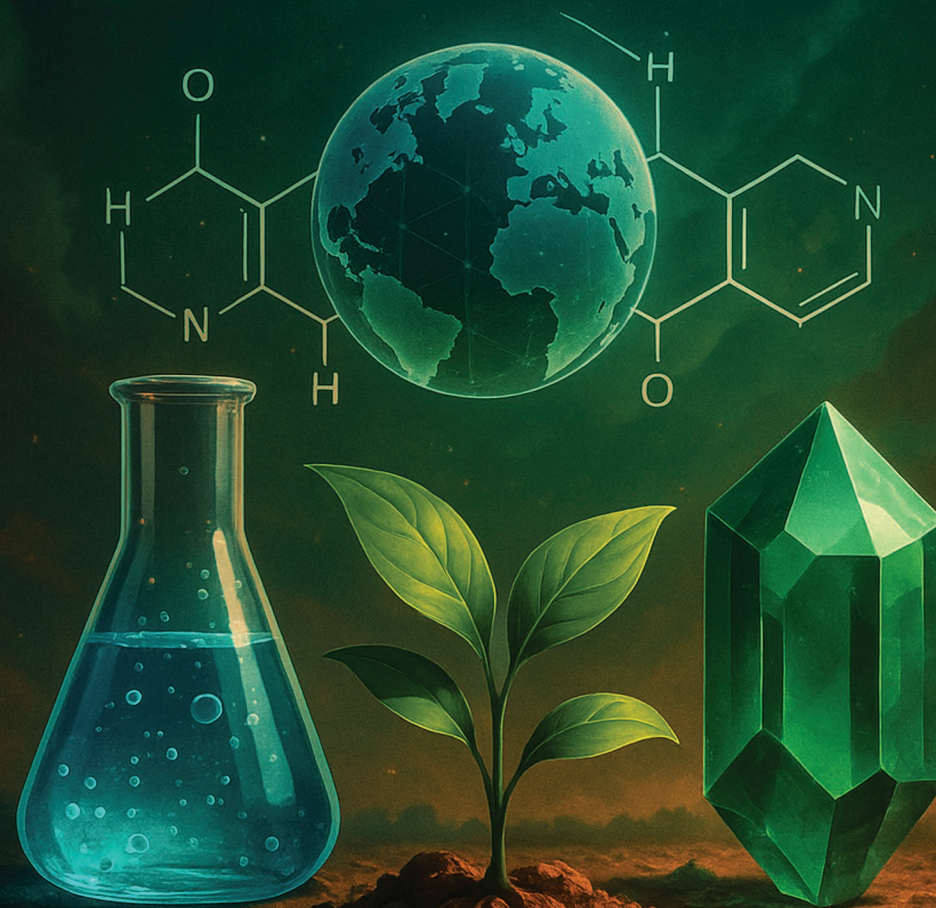
Dr. Naseem Ahmad is an Associate Professor in the Department of Chemistry at Integral University, Lucknow. He completed his Master's degree in Industrial Chemistry from Integral University, Lucknow, and earned his PhD in Industrial Chemistry in 2014 from the same institution. He has over 16 years of teaching and research experience. His research interests primarily focus on medicinal chemistry and nanosciences. Dr. Ahmad is the author and co-author of more than 40 research articles and several book chapters published in reputed national and international journals.



Dr. Firoj Hassan completed his master's degree in industrial chemistry and secured a gold medal in the year 2010 and was selected for INSPIRE fellowship from DST, New Delhi in the year 2011. He has awarded by Ph.D. Degree in Chemistry on the topic "Synthesis of Carbohydrate derivatives as Potential Therapeutic Agents" in the year 2015. Currently, He is working as Assistant Professor in the Department of Chemistry, Integral University, Lucknow, INDIA last twelve years. He has published more than 35 research articles, two patent, one edited book and ten book chapters in reputed journal. Moreover, he has also one year of Industrial experience in Q.C. Department at TATA motors, Lucknow. His research interests included synthetic and medicinal chemistry for the design and development of biologically active heterocyclic compounds.

Perspectives of Medicinal, Material and Environmental Chemistry

PERSPECTIVES OF MEDICINAL, MATERIAL AND ENVIRONMENTAL CHEMISTRY



Editors:
Dr. Saimah Khan
Dr. Naseem Ahmad
Dr. Firoz Hassan



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Perspectives of Medicinal, Material and Environmental Chemistry

Editors

Dr. Saimah Khan

Department of Chemistry, Integral University, India

Dr. Naseem Ahmad

Department of Chemistry, Integral University, India

Dr. Firoz Hassan

Department of Chemistry, Integral University, India



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Published by: - Book Rivers

Website: - <https://www.bookrivers.com>

Email: publish@bookrivers.com

1st Print Edition - 2026

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Title: Perspectives of Medicinal, Material and Environmental Chemistry

Editors: Dr. Saimah Khan, Dr. Naseem Ahmad, Dr. Firoz Hassan

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ISBN: 978-93-6884-556-0

MRP: 400 /-INR

(Printed in India)

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CHAPTER – 6

A Computational Study of Chalcone Derived Cu(II) and Zn (II) Complexes

Supreet¹, Tahmeena Khan¹, Mohammad Imran Ahmad^{1*}

¹*Department of Chemistry, Integral University, Lucknow, Uttar Pradesh,
226026, India*

**Corresponding email: miahmad@iul.ac.in*

Abstract

The simplicity of chalcone chemistry, coupled with the ease of structural modification and straightforward synthesis, has made them a focal point for medicinal chemists exploring a wide range of biological applications. Chalcone derivatives, renowned for their diverse biological activities, have gained significant attention in recent years. In this chapter, we employed computational methods to investigate the physicochemical properties of Cu(II) and Zn(II) complexes derived from various chalcone derivatives which lead to the identification of drug likeness. Computational predictions offer a powerful tool for accelerating drug discovery. By predicting molecular structure, properties, and potential side effects, these techniques can help identify promising lead compounds and optimize their design. Additionally, computational methods can aid in the identification of disease-specific targets, streamlining the development process. Careful consideration of ADMET properties, pharmacokinetics, metabolism, and safety profiles is essential to ensure the clinical viability of these compounds. The results obtained provide insights into the factors influencing the stability, reactivity, and potential biological activity of these metal complexes. This computational study contributes to a deeper understanding of the structure-activity relationships of