

## SYNTHESIS, CHARACTERIZATION, ANTIMICROBIAL STUDIES, AND MOLECULAR DOCKING STUDIES OF TRANSITION METAL COMPLEXES FORMED FROM A BENZOTHIAZOLE-BASED AZO LIGAND

Saud I. Al-Resayes<sup>1</sup>, Amer J. Jarad<sup>2</sup>, Jinan M. M. Al-Zinke<sup>3</sup>, Taghreed H. Al-Noor<sup>2\*</sup>, Marei M. El-ajaily<sup>4</sup>, Mohnad Abdalla<sup>5</sup>, Kim Min<sup>6</sup>, Mohammad Azam<sup>1\*</sup>, Ranjan K. Mohapatra<sup>7\*</sup>

<sup>1</sup>Department of Chemistry, College of Science, King Saud University, Riyadh, 11451, Saudi Arabia

<sup>2</sup>Department of Chemistry, College of Education for Pure Science / Ibn-Al-Haitham, University of Baghdad, Iraq

<sup>3</sup>Department of Chemistry, College of Science, University of Diyala, Iraq

<sup>4</sup>Department of Chemistry, Faculty of Science, University of Benghazi, Benghazi, Libya

<sup>5</sup>Key Laboratory of Chemical Biology (Ministry of Education), Department of Pharmaceutics, School of Pharmaceutical Sciences, Cheeloo College of Medicine, Shandong University, 44 Cultural West Road, Shandong Province 250012, PR China

<sup>6</sup>Department of Safety Engineering, Dongguk University, 123 Dongdae-ro, Gyeongju 780714, Gyeongbuk, Republic of Korea

<sup>7</sup>Department of Chemistry, Government College of Engineering, Keonjhar, Odisha, India

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**ABSTRACT.** The azo ligand obtained from the diazotization reaction of 2-aminobenzothiazole and 4-nitroaniline yielded a novel series of complexes with Co(II), Ni(II), Cu(II), and Zn(II) ions. The complexes were investigated using spectral techniques such as UV-Vis, FT-IR, <sup>1</sup>H and <sup>13</sup>C NMR spectroscopic analyses, LC-MS and atomic absorption spectrometry, electrical conductivity, and magnetic susceptibility. The molar ratio of the synthesized compounds was determined using the ligand exchange ratio, which revealed the metal-ligand ratios in the isolated complexes were 1:2. The synthesized complexes were tested for antimicrobial activity against *S. aureus*, *E. coli*, *C. albicans*, and *C. tropicalis* bacterial species. Additionally, their binding affinities were predicted using molecular docking analysis, and their pharmacokinetic and drug-likeness properties were evaluated.

**KEY WORDS:** Azo ligand, Metal complexes, Antimicrobial studies, Molecular docking study

### INTRODUCTION

Organic molecules with electron donor/acceptor groups containing  $\pi$ -conjugated systems have attracted a lot of interest over the years owing to their unique molecular structure and potential applications [1-6]. Among such compounds, the azo compounds having the C–N=N–C functionality are widely employed as photoactive materials in optics and solar cells, as well as in pharmaceutical and biological research as biochemical sensors, catalysts, and enzyme inhibitors [7-12]. Azo compounds have also been used in coordination chemistry as they display strong chelating ability. The resulting azo ligand-based metal complexes have exceptional thermal stability and have found useful applications in photoelectronics, as dyes in the textile industry, and as scaffolds for the design of new anti-inflammatory, anticancer, and antimicrobial agents [13-17]. In fact, with the rise in antimicrobial drug resistance worldwide, transition metal complexes have gained a lot of attention due to their effectiveness against a range of pathogens [18-21].

\*Corresponding author. E-mail: drtaghreed2@gmail.com; azam\_res@yahoo.com; ranjank\_mohapatra@yahoo.com

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