

ABSTRACT

Complex compounds have various bioactivities influenced by structure and chelation mode from the coordination bond between ligand and metal ion as central atom. Schiff base ligands are ligands with azomethine (C=N) groups synthesized through a condensation reaction between aldehydes/ketones with primary amines. One of the derivatives of Schiff base ligands is salen ligand which capable of forming multidentate chelates producing stable complex compounds. The stability of complex affects its bioactivities such as antibacterial, antifungal, anticancer, and antioxidant. The central metal ion also plays a role in increasing bioactivity. The focus of this research is to synthesize salen ligand derivatives from salicylaldehyde, ethylenediamine, and ortho-vanillin precursors, namely Salenov ligands, and to determine the effect of different metal ions (Ni(II), Cu(II), and Zn(II)) on their antibacterial activity.

Salenov ligands were synthesized from salicylaldehyde, ethylenediamine, and ortho-vanillin in ethanol solvent with a mole ratio of 1:1 refluxed for 4 hours at 80°C then recrystallized and characterized by UV-Vis spectrophotometer, Fourier Transform Infrared (FT-IR), and Nuclear Magnetic Resonance (NMR). Salenov ligands reacted with Ni(II), Cu(II), and Zn(II) metals in methanol with a mole ratio of 1:1 by reflux for 6 hours at 70°C then recrystallized. The complex compounds were characterized using UV-Vis spectrophotometer, Fourier Transform Infrared (FT-IR), Magnetic Susceptibility Balance (MSB), and elemental analysis. The bioactivity of Salenov ligands and complexes was evaluated through antibacterial tests of *Escherichia coli* and *Staphylococcus aureus* with the well diffusion method and compared with computational studies through molecular docking.

The characterization results showed that Salenov ligand was successfully synthesized with the presence of an imine group (C=N) in the infrared spectra. The structure of the Salenov ligand confirmed ¹H NMR and ¹³C NMR characterization. The Ni(II), Cu(II), and Zn(II)-Salenov complexes were also successfully synthesized with the appearance of new peaks in the UV-Vis spectra and a shift in the wave number of imine group (C=N) infrared spectra. From the MSB characterization, square planar geometry was obtained for Ni(II)-Salenov complex and octahedral for Cu(II) and Zn(II)-Salenov complexes. Through elemental analysis, molecular formulas Ni(II), Cu(II), and Zn(II)-Salenov known, respectively, C₁₇H₂₀N₂O₅Ni, C₁₇H₂₀N₂O₅Cu, and C₁₇H₂₀N₂O₅Zn. Antibacterial test *E. coli* and *S. aureus* showed the bioactivity of Salenov complex better than Salenov ligand, where the inhibition of Cu(II)-Salenov was the strongest compared to Ni(II) and Zn(II)-Salenov.

Keywords: Schiff base, complex compound, antibacterial, molecular docking