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Synthesis and characterization of (E)-N-carbamimidoyl -4 and (E)-4- benzenesulfonamides; biological study, DFT, molecular docking, and ADMET predictions

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Sulphonamide Schiff bases (L_1 and L_2) containing imidazole nuclei have been synthesized and evaluated for their antimicrobial and antioxidant activity. Sulfaguanidine and sulfamerazine have been condensed with 4-methyl-5-imidazolecarboxalehyde to obtain ligands L_1 and L_2, respectively. The compounds have been characterized by FT-IR, ^1H and ^{13}C NMR, UV-Vis, CHNS, and MALDI-TOF mass spectral data. The antimicrobial activity of the sulphonamide-derived Schiff bases have been conducted using agar well diffusion against *S. aureus*, *B. substilis*, *E. Coli*, *Salmonella spp.*, and *Candida spp*. Similarly, the free radicals scavenging activity of the compounds has been evaluated at 20 – 100 µg/mL using DPPH (1,1'-diphenyl-2-picryl-hydrazil), nitric oxide, and hydrogen peroxide antioxidant assays. Both compounds exhibited moderate activity against *Salmonella spp*. However, L_1 exhibits higher radical scavenging ability than L_2 against NO free radicals at low to high concentrations with IC_{50} values of 84.50 and 101.59 µg/mL for L_1 and L_2, respectively. Ligand L_2 is however, more active than L_1 against H_2O_2 free radicals at low concentrations (20 – 60 µg/mL). The optimized geometries of the compounds have been docked at the active sites of cytochrome oxidase, myeloperoxidase, NADPH oxidase, xanthine oxidase, dihydropteroate synthase (DHPS), and dihydrofolate reductase (DHFR) proteins.

Keywords: *In silico*, Schiff bases, DPPH assay, Imidazole, Antioxidants, Antimicrobial