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Original Article

Synthesis, Antibacterial Evaluation, and Docking Studies of Some Azo Compounds and Schiff Bases Derived from Sulfonamide

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ABSTRACT

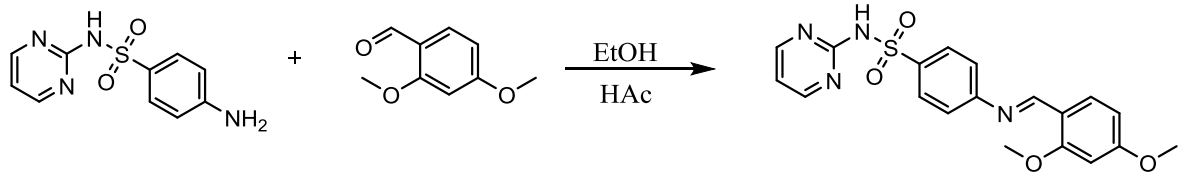
Objective: The aim of study was to synthesize new products of sulfonamide compounds containing azo and Schiff base fragments and confirm the structures by ^{1}H-NMR and FT-IR spectroscopy, as well as to investigate the antibacterial activities against medically important Gram (+) and Gram (-) bacterial strains.

Materials and Methods: Novel sulfonamides derivatives S1, S2, S3, A1, A2, and A3 were synthesized and tested with *staphylococcus aureus* and *Pseudomonas aeruginosa* as well as against *Candida albicans* fungi. Molecular docking was used to study the theoretical binding of the compounds with some selected proteins.

Results: It was found that compounds S1, S2, and S3 have more potent activity against the three types of microorganisms as compared with A1, A2, and A3. Against *Candida albicans*, it was found that compounds S1 and S3 gave the best activity, 21 and 20 mm, respectively. Antibacterial activity showed that compound A2 gave the best activity (34 mm at 1000 µg/mL) against *Staphylococcus aureus*. Other compounds S1, S2, S3, A1, and A3 gave very good activities against the same bacteria, 29, 13, 29, 28, and 28 mm, respectively, at the same concentration. Antibacterial activity against *Pseudomonas aeruginosa* showed that the compounds S1 gave the best inhibition zone (25 mm) at 1000 µg/mL, whereas compounds S2 and S3 showed good potent activity (15 and 20 mm, respectively). Molecular docking studies showed that free binding energy (S) of the compounds against *S. aureus* using protein 1JIJ were -7.15 to -8.60 kcal/mol, whereas free binding energy (S) using 5V5Z fungi protein gave the values -7.10 to -8.22 kcal/mol.

Conclusion: Schiff bases gave good activity against the selected microorganism species compared with azo compounds. There is clear correlation between the activity of the compounds and their molecular docking through the high negative values of free binding energy.

GRAPHICAL ABSTRACT



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