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Studies on the Synthesis of Benzene Sulfonamides, Evaluation of Their Antimicrobial Activities, and Molecular Docking

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SUMMARY. New series of sulfonamides were synthesized and investigated as antimicrobial agents. The structures of newly synthesized compounds were described by IR, ^{1}H and MS spectral data. Antibacterial and antifungal activities were evaluated with ciprofloxacin and itraconazole using disc diffusion method and minimum inhibitory concentration values were determined by 96-well plate assay method. Our studies showed that compounds **13-16** have promising antibacterial against the *S. aureus* having MIC 0.98 μg/mL and IC_{50} ranged between 4.3-10 μg/mL while **16** has promising antifungal activity. clogP was computed to describe the lipophilic character and it was found that the compounds possessing higher clogP have high activity against *S. aureus*. Molecular docking studies of reported compounds were also performed on *S. aureus* dihydropteroate synthase enzyme to identify the plausible binding modes and to explore the binding mechanism of these compounds.

RESUMEN. Se sintetizaron e investigaron nuevas series de sulfonamidas como agentes antimicrobianos. Las estructuras de los compuestos recién sintetizados se describieron mediante datos espectrales IR, ^{1}H y MS. Las actividades antibacterianas y antifúngicas se evaluaron con ciprofloxacina e itraconazol utilizando el método de difusión en disco y los valores de concentración mínima inhibitoria se determinaron mediante el método de ensayo en placa de 96 pocillos. Nuestros estudios mostraron que los compuestos **13-16** tienen prometedor acción antibacteriana contra *S. aureus,* con MIC 0,98 μg/mL e IC_{50} osciló entre 4,3-10 μg/mL, mientras que **16** tiene una actividad antifúngica prometedora. clogP se calculó para describir el carácter lipofílico y se descubrió que los compuestos que poseen mayor clogP tienen una alta actividad contra *S. aureus*. Los estudios de acoplamiento molecular de los compuestos informados también se realizaron en la enzima dihidropteroato sintasa de *S. aureus* para identificar los modos de unión plausibles y explorar el mecanismo de unión de estos compuestos.

KEY WORDS: bacterial strains, IC_{50}, MIC, molecular docking, sulfonamides.

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