Indian Journal of Heterocyclic Chemistry
Vol. 31 - Number 03 (Jul-Sep 2021) 405-416
DocID: https://connectjournals.com/01951.2021.31.405

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis, Computational Docking, and Antimycobacterial Study of Novel *N'*-phenyl-4-pyrrol-1-yl-benzenesulfonamide Derivatives

Yahya S. Alqahtani[1], S. R. Prem Kumar[2], H. Pavitra[2], Shrinivas D. Joshi[2]*

[1]Department of Pharmaceutical Chemistry, College of Pharmacy, Najran University, Najran, Saudi Arabia
[2]Department of Pharmaceutical Chemistry, Novel Drug Design and Discovery Laboratory, Soniya Education Trust's College of Pharmacy, Sangolli Rayanna Nagar, Dharwad, Karnataka, India

ABSTRACT Fresh sequences of pyrrole linked *N*'-phenyl-4-pyrrolyl-benzenesulfonamide derivatives were synthesized by different synthetic methods. Synthesis of the *N*'-phenyl-4-(1*H*-pyrrol-1-yl) benzenesulfonamides **5(a-e)**/4-(2,5-dimethyl-1*H*-pyrrol-1-yl)-*N*'-phenylbenzenesulfonamides **6(a-e)** was achieved by refluxing 2,5-dimethoxytetrahydrofuran/hexane 2,5-dione separately in presence of acetic acid. Further, synthesis of *N*-(4-(*N*'-phenylsulfamoyl)phenyl)-4-(1*H*-pyrrol-1-yl)benzamides **8(a-b)**/4-(2,5-dimethyl-1*H*-pyrrol-1-yl)-*N*-(4-(*N*'-phenylsulfamoyl)phenyl)benzamides **10(a-b)** was achieved by cold stirring of 4-(1*H*-pyrrol-1-yl)benzoic acid **(7)**/2,5-dimethyl-1*H*-pyrrol-1-yl)benzoic acid **(9)** correspondingly in the presence of 2-(1*H*-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate, *N', N'*-diisopropylethylamine, and Dimethylformamide. *In vitro* anti-tubercular study of afresh compounds has shown good minimum inhibitory concentration values (**0.4–12.5** μg/mL) counter to *Mycobacterium tuberculosis* H_{37}Rv, while the corresponding study of reported molecules for antibacterial activity disclosed considerable inhibition values (**0.4**–**25** μg/mL) counter to *Escherichia coli* (Gram–ve) than *Staphylococcus aureus* (Gram +ve).

KEYWORDS Pyrrolyl-sulfonamides, Docking study, *Mycobacterium tuberculosis* H_{37}Rv, Antibacterial activity.

How to cite this article: Alqahtani, Y.S, Kumar, S.R.P., Pavitra, H., Joshi, S.D. Synthesis, Computational Docking and Antimycobacterial Study of Novel *N'*-phenyl-4-pyrrol-1-yl-benzenesulfonamide Derivatives, *Indian J. Heterocycl. Chem.*, **2021**, *31*, .405–416. *(DocID: https://connectjournals.com/01951.2021.31.405)*