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Synthesis , in -Vitro and in Silico studies of azo-based calix [4]arenes as antibacterial agent and neuraminidase inhibitor: A new look into an old scaffold (Article) (Open Access)

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Abstract

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Calixarene derivatives are reported as potential therapeutic agents. Azo derivatives of calixarenes have not been given much consideration to explore their biomedical applications. In the present study, some azo-based derivatives of calix[4]arene were synthesized and characterized and their antibacterial and antiviral potentials were studied. The mono azo products of sulphanilamide, sulfaguanidine and 2-methyl-4-aminobenzoic acid showed good activity against bacterial strains with minimum inhibition concentration values ranging from 0.97 to 62.5 μg/mL. For mono azo products, the diazotized salt was applied as a limiting reagent. The use of calix[4]arene and sodium acetate trihydrate in 1:3 (molar ratio) helped in partial substitution. Molecular docking was performed to see the interaction of the designed compounds with two bacterial and one viral (neuraminidase) receptor. Some of the derivatives showed good interaction with the active site of bacterial and neuraminidase enzymes through hydrogen, hydrophobic and pi-pi interactions, and could inhibit the activity of the selected enzymes. © 2018 Ali, Muhammad Bunnori, Susanti, Muhammad Alhassan and Abd Hamid.

SciVal Topic Prominence

Topic: synthesis | Metal ions | Conformations

Prominence percentile: 84.6

Reaxys Database Information

View Compounds

Author keywords

Antibacterial activity | Azo calix[4]arenes | Calix[4]arenes | Docking | Neuraminidase inhibition

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