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Synthesis and molecular docking of 2,4,5-trisubstituted-1,3-thiazole derivatives as antibacterial agents (Article) [\(Open Access\)](#)

[Sintesis dan penyatuan molekul terbitan 1,3-tiazol berpenggantian- 2,4,5 sebagai agen antibakteria]

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Abstract

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The emergence of antibiotic resistance against bacterial strains has attracted great interest in the discovery and development of new antibacterial agents. Thiazole derivatives have been widely used in the biological as well as pharmacological fields and their efficiency as pharmaceutical drugs are well established. In this study, a series of thiazole derivatives were synthesized in reaction between 3-chloroacetyl acetone and ammonium thiocyanate followed by incorporating selected amines in one-pot synthesis manner. The compounds were structurally characterized by Fourier Transform Infrared (FTIR), Proton Nuclear Magnetic Resonance (¹H NMR), Ultraviolet-Visible (UV-Vis) and Gas Chromatography-Mass Spectrometry (GC-MS). Their antibacterial properties were screened using disc diffusion technique against selected Gram-positive (*Bacillus cereus* and *Staphylococcus epidermidis*) as well as Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*) with T₃ exhibited the most potent antibacterial activity. Molecular docking studies were also performed against Glucosamine-6-phosphate (GlcN-6-P) synthase which is known as the essential building block of most bacteria. The docking result displayed that T₃ exhibited the minimum binding energy of -7.09 kcal mol⁻¹ as compared to T₁ and T₂ with -6.49 and -6.76 kcal mol⁻¹, respectively which is in agreement with antibacterial result. The output of this preliminary study will contribute in structural enhancement in drug discovery. © 2019, Malaysian Society of Analytical Sciences. All rights reserved.

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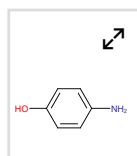
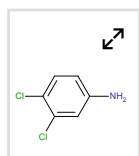
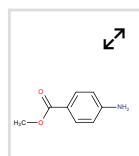
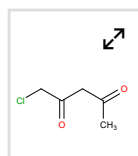
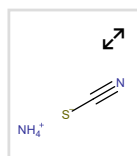
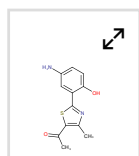
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