Prospecting carbonic anhydrase as a drug target for antibiotic resistant *Vibriocholerae* infection management: An *in silico* approach

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ABSTRACT

Vibrio cholerae, a Gram-negative bacterium that causes cholera, reported worldwide has developed significant antibiotic resistance. CA inhibitor was recently demonstrated to inhibit the bicarbonate-mediated virulence induction in *V. cholerae*. Moreover, CA was identified as druggable targets in several pathogenic bacteria. In this work, crystal structure of beta carbonic anhydrase from *Vibrio cholerae* [PDB ID: 5CXK] was retrieved from Protein data bank. The Auto Dock Vina tool was used for screening thirty-eight selected phytochemical compounds with carbonic anhydrase inhibition property. The compounds were ranked based on the binding energy value and three compounds with highest binding energy was chosen for further analysis. Xenosite prediction, Mol inspiration, and QSAR (Quantitative Structure Activity Relationship) models were used to predict the toxicity of three compounds. Based on the molecular docking, Morelloflavone (-6.9 Kcal/mol) and Vokensiflavone (-6.9 Kcal/mol) were found to have better docking score with 5CXK. This was followed by Baicalin (-6.8Kcal/mol). The amino acid residues involved in interactions using hydrogen bonding were Gln A:6 in Morelloflavone and Arg B: 194 and Arg H:131 in Vokensiflavone. Apart from hydrogen bonding, other interactions found were pi-sigma, pi-alkyl, and C-H bonds. Based on the toxicity analysis using T.E.S.T software and QSAR model, these compounds were found to be a safer drug molecule that could be used as a potential carbonic anhydrase inhibitor. To conclude, these phyto-compounds could act as an effective drug molecule with lower toxicity to overcome the antibiotic resistance in *Vibriocholerae* infection management.

Keywords: Carbonic anhydrase; Cholera; phytomedicines; molecular docking

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