INHIBITION STUDY BY MOLECULAR DOCKING OF DIHYDROFOLATE REDUCTASE OF *ESCHERICHIA COLI* WITH SOME CHALCONE MOLECULES

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ABSTRACT

A série of chalcone was synthesed by catalysed claisen schmit condensation and evalated for biological activity against a various micro-organisme such *Staphylococcus aures ATCC, Klebsiela pneumonia ATCC, Escherichia Coli ATCC, Pseudomonas aeruginosa ATCC* using the disk diffusion method and the minimum inhibitory concentration (MIC). Molecular modeling (docking) studies show that 4,4'methyl méthoxychalcone represents the best inhibitor for the *E.coli* dihydrofolate reductase (4DHFR). The crystals of the compound **Ib** were successfully grown by the solution growth technique at room temperature. Single crystal XRD studies indicated the orthorhombic structure of *(E)-3-(2,6-Dichlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one*.

KEYWORDS: Chalcones, Biological Activity, MIC, Dihydrofolate Reductase, X-Ray Diffraction