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Design and Synthesis of Novel Methylenedioxyphenyl Derivatives as Potential Anticancer Agents †

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Abstract: Methylenedioxyphenyl and its derivatives are found in natural products, including safrole and drugs such as tadalafil, MDMA, paroxetine, and piperonyl butoxide. It is one of the important pharmacophores of podophyllotoxin and exhibits remarkable anticancer potential by inhibiting the enzyme Topoisomerase II. Naturally occurring podophyllotoxin has limited resources, so, therefore, there is a need to develop synthetic derivatives which may fulfill the demand. In the present work, we have designed and synthesized methylenedioxyphenyl derivatives. Molecular docking approaches are routinely used in modern drug design to help understand the drug-receptor interaction. Docking studies of methylenedioxyphenyl derivatives were performed with the help of AutoDock Vina software to reveal the interactions of these compounds with the active sites of DNA Topoisomerase-II with the PBD ID 1ZXN. These methylenedioxyphenyl derivatives were synthesized by using Claisen-Schmidt condensation, followed by a cyclization reaction. Then, these derivatives were characterized by Infrared and Nuclear Magnetic Resonance spectroscopy. When docked, maximum derivatives of the designed series showed the best possible binding site to inhibit DNA topoisomerase II with Gibbs free energy in between the range of -8.8 and -9.5 kcal/mol. Compounds show common van der Waals interactions to residues GLY160, GLY164, GLY166, and MG900. Thereby, whole studies served as a basis for developing better potential therapeutic compounds for anticancer activity.

Keywords: methylenedioxyphenyl; DNA Topoisomerase II; podophyllotoxin; anticancer; AutoDock Vina; molecular docking.

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Conflicts of Interest

The authors declare no conflict of interest.