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Molecular docking and dynamic simulation of anti-apoptotic BCL-2 with saponins isolated from *Weigela* x "Bristol Ruby"

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Colon cancer is the second leading cause of cancer-related deaths worldwide. Apoptosis may play a key role in the tissue mass homeostasis of the colonic mucosa. The B-cell lymphoma-2 (BCL-2) family plays an important role in determining the decision to undergo apoptosis. A previous study revealed the potential cytotoxicity on colorectal cancer cell line of triterpenoid saponins isolated from *Weigela* x "Bristol Ruby". In this *in silico* study, triterpenoid saponins from *W.* x "Bristol Ruby" have been studied for their inhibition potential using molecular docking on the 6GL8 receptor. All compounds exhibit hydrogen bonds, Van der Waals, and hydrophobic interactions in molecular docking. The binding potentials of triterpenoid saponins and a reference compound, 5-FU, as target protein 6GL8 have been examined using molecular docking. Among of those, 3-*O*-β-D-xylopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)-β-D-xylopyranosyl-(1→3)-α-L-rhamnopyranosyl-(1→2)-α-L-arabinopyranosyloleanolic acid (CPD1) binds to the 6GL8 receptor with the highest binding stabilities at –5.08 kcal/mol, in comparison with the reference 5-FU at –3.59 kcal/mol. Molecular dynamic studies have been further conducted to better comprehend ligands' dynamics within the target protein's binding pocket. The result show that the binding of CPD1 to the 6GL8 receptor is stable throughout the simulation. CPD1 could be a good candidate for new inhibitors of anti-apoptotic BCL-2 proteins in colorectal cancer.

Keywords: Colorectal cancer, *Weigela* x "Bristol Ruby", Molecular docking, Molecular dynamic simulation, Triterpenoid saponin