Targeting Bcl-2 anti-apoptotic receptor with gossypetin from *Moringa oleifera*: An in-silico study for colorectal cancer prevention

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Abstract

Colorectal cancer (CRC), the most lethal form of cancer in humans, is brought on by an accumulation of genetic material damage that results in unregulated cell growth in the large intestine. Despite the fact that various chemotherapy medications have been documented for colorectal cancer, their lack of safety, effectiveness, and selectivity make them ineffective. Therefore, it is quite admirable that there are new alternative anticancer drugs that work so well. Numerous bioactive chemicals found in natural plants have long been utilized for various kinds of medicinal purposes. Gossypetin, in particular, is a naturally occurring bioactive substance that is frequently present in *Moringa oleifera* and has demonstrated a variety of biological functions. We have examined the expression of the apoptosis blocker Bcl-2 and the proapoptotic proteins Bak and Bax since the role of the Bcl-2 gene family in colorectal cancer has not been fully investigated. Recent research has demonstrated that Bcl-2 gene receptors are expressed in a number of cancers, including colorectal cancer, making them potential targets for treatment development. The binding affinity, stability, and drug likeness characteristics of the top-ranked screened compounds and gossypetin were ascertained in the current in silico study using structure-based virtual screening, molecular docking, molecular dynamics simulation, and Adsorption, Distribution, Metabolism, Excretion (ADME) prediction. The screened compounds violated the drug similarity qualities, although the findings showed that the complex had strong molecular interactions, binding stability (peak between 0.3 and 0.4 nm), and no violations in the Lipinski Rule of 5 in gossypetin. The gossypetin molecule may help create a potential treatment strategy against colorectal cancer, according to the *in-silico* analysis.

Keywords: Bcl-2 gene receptor, Colorectal cancer, Docking, Gossypetin, Receptor–ligand interactions, Tumor targeting

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