ABSTRACT

Colorectal cancer is one of the most common cancers worldwide, and it is also one of the major causes of mortality from cancer. Chemotherapy drugs are generally limited due to various complications, as well as the development of resistance and recurrence. The in silico docking investigation involved exploration of protein or nucleotide, 3D structural modeling, molecular docking, and binding energy calculation. Protein-protein interactions are significant to many biological processes, and their disruption is a leading cause of disease. The use of small molecules to modulate them is gaining popularity, but protein interfaces usually lack specific cavities for processing small molecules. MMP-2, PARP, iNOS, Chk1, proteins were used in the molecular docking analysis of kaempferitrin and 5-flurouracil. The compound kaempferitrin had the highest binding energy scores with most of the target proteins, according to molecular docking results. The findings suggest it could be used to develop new drugs for cancer therapy.