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Abstract	:	Colorectal cancer (CRC) is notoriously known as the third most common cancer worldwide, and the fourth common cause of death caused by cancer with 700,000 deaths per year. CRC incidence rates were observed to be rising in developing countries including Malaysia, as it was reflected by increased prevalence of risk factors for CRC that are associated with westernization such as unhealthy diet, obesity and smoking prevalence. The fungus family Cordyceps spp. has long been explored in the Traditional Chinese Medicine (TCM) as food, tonic and folk medicine to treat diseases ranging from malaria to cancer. Cordycepin, an active component in Cordyceps militaris were shown to have the anticancer and antimetastatic effect related to its adenosine and its derivatives. In current study, cordycepin inhibitory property against several CRC biomarkers was explored in-silico. Molecular docking and dynamics study of cordycepin against 6 important CRC biomarkers, namely caspase-3, caspase-8, COX-2, IL-2 and IL-6 were performed and its affinity was compared with obatoclax, a Phase II clinical trial antitumor drug which induces apoptosis in cancer cells by functioning as an inhibitor for Bcl-2 family proteins. The result shows that cordycepin is able to act as inhibitors for the selected CRC biomarkers, with equivalent or higher affinity compared to obatoclax. The in-silico prediction study provides a screening platform for the development of anti-CRC drug based on the Cordyceps spp., and in addition, provides a protocol to minimize the laboratory toxicological hazard and promotes the application of green chemistry computing in the drug discovery research.