

Abstract

Exploratory Studies on Anticancer Potential of a Vernonia Species against Colorectal Adenocarcinoma: In Vitro Studies and In Silico Mechanistic Investigations [†]

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Abstract: Globally, colorectal cancer (CRC) is amongst the most prevalent cancer incidences, being the second most common amongst women and third most common amongst men as revealed by 'GLOBOCAN 2022' statistics. The projected morbidity for CRC is more than 3 million by the year 2040 according to the 'WHO Cancer Tomorrow' predictions. Surgery, chemotherapy, and radiation therapy continue to be the primary treatment options, each with particular limitations. There is a growing need for identification of alternate therapies for the treatment of colorectal cancer to overcome the shortfalls of these treatment options. Phytoconstituents offer diverse pharmacophoric scaffolds with unique chemical features. In this work, successive extracts of aerial plant parts of a Vernonia species (family Asteraceae) have been screened in vitro on colorectal adenocarcinoma cell lines Colo205 and HT-29 by MTT assay and compared with 5-Fluorouracil as the reference standard. The plant is known to possess triterpenoids, quaternary alkaloids, phenolics, and sesquiterpene lactones. In silico docking studies have been carried out on the plausible phytoconstituents of the active extracts against vital protein targets involved in the progression of CRCs, such as cyclin-dependent kinases, and enzymes of apoptotic pathways, such as caspases, etc. These studies will help to discover the mechanistic details of the anticancer activity of the plant and will provide a platform for the development of novel multi-targeted small molecules.

Keywords: colorectal cancer; phytoconstituents; Vernonia; docking; proteins



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