World Academy of Science, Engineering and Technology
International Journal of Biotechnology and Bioengineering
Vol:17, No:05, 2023

In-silico Target Identification and Molecular Docking of Withaferin A and Withanolide D to Understand their Anticancer Therapeutic Potential

Authors : Devinder Kaur Sugga, Ekamdeep Kaur, Jaspreet Kaur, C. Rajesh, Preeti Rajesh, Harsimran Kaur

Abstract : Withanolides are steroidal lactones and are highly oxygenated phytoconstituents that can be developed as potential anti-carcinogenic agents. The two main withanolides, namely Withaferin A and Withanolides D, have been extensively studied for their pharmacological activities. Both these withanolides are present in the Withania somnifera (WS) leaves belonging to the family Solanaceae, also known as “Indian ginseng .”In this study effects of WS leaf extract on the MCF7 breast cancer cell line were investigated by performing a 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT) assay to evaluate the cytotoxic effects and in vitro wound-healing assay to study the effect on cancer cell migration. Our data suggest WS extracts have cytotoxic effects and are effective anti-migrating agents and thus can be a source of potential candidates for the development of potential agents against metastasis. Thus, it can be a source of potential candidates for the development of potential agents against metastasis. Insight into these results, the in-silico approach to identify the possible protein targets interacting with withanolides was taken. Protein kinase C alpha (PKCα) was among the selected 5 top-ranked target proteins identified by the Swiss Target Prediction tool. PKCα is known to promote the growth and invasion of cancer cells and is being evaluated as a prognostic biomarker and therapeutic target in clinically aggressive tumors. Molecular docking of Withaferin A and Withanolides D was performed using AutoDock Vina. Both the bioactive compounds interacted with PKCα. The targets predicted using this approach will serve as leads for the possible therapeutic potential of withanolides, the bioactive ingredients of WS extracts, as anti-cancer drugs.

Keywords : withania somnifera, withaferin A, withanolides D, PKCα
Conference Title : ICABB 2023 : International Conference on Advanced Bionanotechnology and Biomaterials
Conference Location : Montreal, Canada
Conference Dates : May 15-16, 2023