SUMMARY

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Chapter 1: Screening of Selected Medicinal Plants; Qualitative and Quantitative Phytochemical Analysis

This chapter summarised that the plants were selected based on their folklore and medicinal significance. Careful consideration was given to ensure diverse species with rich cultural and healing value. This meticulous selection aimed to conserve traditional knowledge and exploit the therapeutic potential of these plants for various purposes. While the anticancer potential of these plants remains underexplored, their historical use in traditional medicine suggests promising anticancer properties. Further studies are required to investigate and authenticate these potential benefits, potentially paving the way for developing novel treatments or therapies explained in remaining chapters.

According to the studies performed in this chapter, can be summarized that, in case of overall screening of four selected plant extracts, Sv leaf extract stands out as a promising natural anti-oxidant, boasting a high concentration of phenols and flavonoids compared to other extracts.

Chapter 2: Anti-proliferative and Cytotoxicity Evaluation of Plant Extracts

Deeper mechanical insights of action of the active compounds from Sv needs to be deciphered to fully understand its potential in cancer therapy. The identification of this compounds and its cytotoxic activity in cancer cells paves the way for future studies to explore the development of novel anti-cancer drugs derived from natural sources.

The anti-proliferative and cytotoxicity activity explained in this chapter summarises, that amongst all extract, Sv leaf aqueous extract has good anti-proliferative activity against MCF-7 cell line while leaf methanolic extract were showing promising anti-proliferative activity against MDA-MB-231 cells without showing any toxicity study on HEK-293 at lower dosage. For upcoming in vitro studies, Sv leaf extract dosage and time durations were considered.

Chapter 3: Chemical composition analysis of *S. virginianum* leaf extract: Unveiling phytochemical diversity

This chapter presents the screening of potential bioactive compounds from Sv leaf extracts through GC-MS and HR-LCMS/MS analysis. Among the more than 30 phyto-compounds identified, nine were selected based on previous literature on studies on breast cancer cell lines. These selected phyto-compounds underwent further in-silico analysis, as detailed in Chapter 4.

Chapter 4: Elucidating the molecular interactions of selected secondary metabolites from *S. virginianum* leaf extracts: Insights from molecular docking and apoptotic marker analysis

This study marks the first assessment of nine specific phyto-compounds through molecular docking experiments. The comprehensive in-silico investigation reveals that Ritterazin A exhibits a favourable binding affinity towards selected cancer sites, positioning it as a potential candidate for future breast cancer therapies. The in-silico findings substantiate the anti-proliferative effects of Sv leaf extracts on MCF-7 and MDA-MB-231 cell lines. Subsequent chapters delve into apoptotic activity via in-vitro tests and molecular research. Numerous docking analyses for specific phytocompounds and melatonin could be pursued.

Chapter 5: Enhancing Anti-Proliferative and Cytotoxic Activity: Exploring Melatonin Alone and in Combination with *S. virginianum* Leaf Extract

In the present study, observations indicated that the sub lethal doses ($IC_{50/2}$) combination and IC_{50} combination of Sv leaf extract and melatonin showed promising reductions in cell viability at 24 hr of exposure. These combinations (extract/melatonin) and exposure duration (24 hr) were considered for further assays (Chapter 6 and 7).

Overall, findings of this chapter highlight the presence of active molecule in the extracts and the combination of it with melatonin shows a novel and effective strategy in cancer treatment. Thus, to unleashed the active principal components present in the plant extracts, next chapter deals with understanding the diversity of it through analytical methods.

Chapter 6: Unlocking Anti-metastatic and Apoptotic Potential: Melatonin and *S. virginianum* leaf Extract Combinations in Breast Cancer Cell lines

The overall results highlight the potential of Sv leaf extract and melatonin in combination to inhibit cell migration and colony formation, induce apoptosis, and affect nuclear morphology in breast cancer cells. The combined treatment at sub-IC_{50} concentrations led to significantly increased apoptotic activity compared to individual treatments, emphasising the synergistic effects of these compounds and their potential for enhanced therapeutic outcomes when administered together.

Chapter 7: Deciphering Anti-Cancer Pathways: Molecular gene expression and bioinformatics analysis of protein-protein interaction of *S. virginianum* Leaf Extract and Melatonin in Breast Cancer Cells

The overall highlights of this chapter shows the multi-faceted effects of the treatments on breast cancer cells, including the induction of apoptosis, inhibition of metastatic potential, and modulation of the immune microenvironment. In summary, the mRNA expression data provide

compelling evidence for the anti-cancer effects of Solanum virginianum plant extract, melatonin, and their combination, underscoring their potential as novel therapeutic agents for breast cancer.

FUTURE POSSIBILITIES

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The findings of our present study suggest the potential use of a combinational approach involving *Solanum virginianum* (*Sv*) leaf extract and melatonin in breast cancer therapeutics. In this regard, we propose the following areas for potential future studies:

- HPLC and advanced separation techniques may be employed to evaluate the different active metabolites present in *Sv* leaf extract through effective fractionation.

- Multiple ligand molecular docking analyses can be conducted to gain deeper insights into the mechanism of action of the combinational therapeutic approach through *in silico* studies.

- *In-vivo* studies using animal models may be carried out to evaluate the anti-cancer activity of the combinational groups (*Sv* leaf extract and melatonin).

- Clinical trials involving human volunteers can be conducted to assess the pharmacological properties of the combinational group (*Sv* leaf extract and melatonin).

- The potential effect shown by phytochemicals in presence of melatonin needs to be understood in terms of their mode of action. (Additive or Complimentary).

These proposed areas of study aim to build upon our current findings and further explore the potential efficacy and mechanisms of action of the *Sv* leaf extract and melatonin combination in breast cancer treatment.