Name of Scholar: **Anam Beg** Name of Supervisor: **Prof. Rafat Parveen** Name of Co-Supervisor: NA Name of Department: **Computer Science** Topic of Research: **Modeling of Gene Regulatory Networks for Druggable Targets of Ovarian Cancer and finding its Potential Inhibitor**

Findings

Ovarian cancer is the most prevalent form of cancer making it the leading cause of mortality among all gynecological malignancies. A growing body of research has demonstrated a correlation between miRNAs and their associated genes in the advancement of ovarian cancer. The present research work aimed to investigate the identification of miRNAs and their associated genes that have a crucial role in the early prediction of patients diagnosed with ovarian cancer. The microarray dataset GSE119055 utilized in this work was obtained from the public GEO database to conduct the modeling of networks and analysis of differentially expressed genes (DEGs).

The network analysis findings revealed the identification of miRNA and its corresponding hub genes from the ovarian cancer samples. The analysis of the network and its associated genes revealed the identification of the top 5 upregulated miRNAs, namely hsa-miR-130b-3p, hsa-miR-18a-5p, hsa-miR-182-5p, hsa-miR-187-3p, and hsa-miR-378a-3p. Additionally, the top 5 downregulated miRNAs, namely hsa-miR-501-3p, hsa-miR-4324, hsa-miR-500a-3p, hsa-miR-1271-5p, and hsa-miR-660-5p, were also identified. Among these miRNAs, a set of 7 common genes (SCN2A, BCL2, MAF, ZNF532, CADM1, ELAVL2, ESRRG) were found to be hub genes in the downregulated

network. Similarly, for the upregulated miRNAs, two hub genes (PRKACB, TAOK1) were identified.

The validation analysis conducted using GEPIA2 confirmed the validity of five genes. However, the results obtained from the KM plotter analysis suggested that out of these five genes, only four exhibited statistical significance. These four genes were subsequently examined for the highest mutation count. ELAVL2 has been made to identify potential therapeutic candidates 2 using a small molecular drug complex. Five compounds, ZINC03830554, ZINC03830332, ZINC03830328, ZINC03830649, and ZINC03831622 were identified. Overall, results of molecular dynamics simulation suggest that the ELAV-like protein 2-ZINC03830554 complex was relatively stable during the simulation. The combined findings suggest that ELAVL2, together with their genetic changes, can be investigated in therapeutic interventions for precision oncology, leveraging early diagnostics and target-driven therapy in ovarian cancer.

Keywords

Ovarian Cancer Differentially Expressed Genes Gene Regulatory Network Molecular Docking MD Simulations