**Supp. Table 2** The significant results obtained in the study are summarized.

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| --- | --- |
| Analysis | Results obtained |
| Differential Gene Expression | * 1085 DEGs were obtained.
* 589 DE mRNAs were identified.
* 496 DE lncRNAs were identified
 |
| PPI Network construction and Hub Gene Identification | * PPI network consisted of 589 nodes and 1036 edges with a clustering coefficient of 0.23.
* 19 clusters were identified from the network, and a significant one with 20 nodes.
* The top 5 hub genes were revealed (CKS1B, CDC25C, IRF1, IFNB1, CDT1).
 |
| GO and Biological Processes | * The hub genes were enriched to the dysregulation of cancer immune response, cell cycle, and post-regulation of the cell cycle.
 |
| Clinical Significance of the Hub Genes | * CKS1B, CDC25C, IRF1, and CDT1 possessed HR > 1.
* Lower median values in the expression groups revealed their expression cohort in NSCLC.
 |
| Co-Expression analysis | * ENST00000605056 lncRNA was upregulated and exhibited the maximum interactions with three highly ranked hub genes (CKS1B, IRF1, and IFNB1).
 |
| Molecular Docking | * A significant bonding interaction between the selected volatile ligands and the lncRNA was observed, primarily through non-covalent bonds.
 |
| Molecular Dynamics Simulation | * In contrast to the control, the complexes acquired conformational stability in the 20 ns trajectory period.
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