**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. |