**Supp. Table 1.** The bioinformatics tools employed in this study and their principles and applications are listed.

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| --- | --- | --- |
| **Analysis** | **Bioinformatics Tools** | **Principle and Applications** |
| Differential Gene Expression | GEO2R-GEO | Compares gene expression profiles in Gene Expression Omnibus (GEO) datasets and identifies differentially expressed genes. |
| Network Construction and Analysis | STRING (<https://string-db.org/>) and Cytoscape | STRING is a database for protein-protein interactions, and Cytoscape is a tool for visualizing and analyzing biological networks. |
| Hub Gene Identification | CytoHubba app of Cytoscape | Identifies hub nodes in biological networks, aiding in identifying key proteins or genes with critical roles in biological processes or diseases. |
| Functional Enrichment | ShinyGO (<http://bioinformatics.sdstate.edu/go/>) | Provides a graphical visualization of enriched GO terms and facilitates the interpretation of large-scale transcriptomics or proteomics data. |
| Clinical Significance | Kaplan-Meier (KM) plotter (<https://kmplot.com/analysis/>) | Performs survival analysis on gene expression data to assess the impact of specific genes on patient survival in various cancers, aiding in identifying prognostic biomarkers. |
| Co-Expression analysis | diffcoexp package of R | Identifies differentially co-expressed gene pairs from transcriptomics data, providing insights into changes in gene co-expression patterns under different conditions or in different samples. |
| RNA Structure Prediction | RNAfold (<http://rna.tbi.univie.ac.at/cgi-bin/RNAWebSuite/RNAfold.cgi>) and RNAComposer (<https://rnacomposer.cs.put.poznan.pl/>) | RNAfold predicts the secondary structure of RNA molecules based on thermodynamic principles, and RNAComposer predicts three-dimensional models of RNA molecules based on their secondary structure and experimental data. They aid in studying RNA structure-function relationships and RNA-based therapeutics. |
| Pharmacokinetic profiling | SwissADME (<http://www.swissadme.ch/>) | Calculates small molecules' physicochemical and pharmacokinetic properties to assess their drug-likeness and suitability for oral bioavailability, aiding drug discovery and optimization. |
| Molecular Docking | HADDOCK 2.4 (<https://wenmr.science.uu.nl/haddock2.4/>) | It is software for molecular docking to determine the structure and energetics of the complexes, aiding in drug discovery. |
| Molecular Dynamics Simulation | GROMACS | It is a molecular dynamics simulation software that determines the behaviour of complex biological systems over time, aiding in understanding the interactions and stability. |