

Abstract Submission No.: A-1043**The Molecular Basis and Potential Drug Prediction for The Co-occurrence of Chronic Kidney Disease and Tuberculosis****Siqin Yi**¹, Ieping Liu², Qiongjing Yuan³¹Department of Internal Medicine-Nephrology, Xiangya Hospital Central South University and Central South University Xiangya School of Medical²Department of Internal Medicine-Nephrology, Xiangya Hospital Central South University²Department of Internal Medicine-Nephrology, Third Xiangya Hospital Of Central South University

Objectives : Chronic Kidney Disease (CKD) is a major health issue with a higher risk of comorbidity with tuberculosis (TB), however, the relationship between the two conditions remains unclear. We decided to use bioinformatics to explore the differentially expressed genes (DEGs) and protein signaling pathways of the co-occurrence of chronic kidney disease and tuberculosis and to provide guidance for treatment.

Methods : We obtained RNA-seq datasets GSE66494 and GSE107991 from GEO and preprocessed the datasets using Bioconductor. We obtained common differentially expressed genes for chronic kidney disease and tuberculosis. We conducted Gene Ontology and pathway enrichment analyses to determine the biological functions and pathways. We used the STRING database and Cytoscape to construct protein-protein interaction network analysis, which identified hub genes. According to hub genes, we predicted potential drugs for the treatment of the diseases. Using Autodock Vina, we performed molecular docking and molecular dynamics simulations for each drug and small molecule pair to identify the combinations with the lowest binding energy.

Results : Through RNA-seq datasets of the GEO database, we identified 30 common differentially expressed genes between the two. The pathway analysis shows that DEGs are significantly enriched in immune-related pathways, including IFN gamma signaling pathway, interferon Alpha/Beta Signaling. GO analysis shows that the DEGs have diverse biological functions, including myosin light chain binding, heme binding. The PPI network includes 30 differentially expressed genes and 10 interaction relationships. IFI6, STAT1, IFIT1, and TNFSF10 were detected as hub genes. The predicted potential drugs are suloctidil, acetohexamide, mefloquine, prochlorperazine, thioridazine, and propofol. Molecular docking showed that the combination with the smallest binding energy was IFIT1 and mefloquine.

Conclusions : This study used bioinformatics to analyse their biological functions of chronic kidney disease and tuberculosis and predicted related drugs, providing important guidance for the treatment of CKD-TB and laying the foundation for future drug research.