Supplementary

Table S1 Primer sequences for genes

Gene	Direction	Primer sequence (5'-3')
β-Actin	Forward	AATCTGGCACCACACCTTCTACAA
	Reverse	GGATAGCACAGCCTGGATAGCAA
GSTP1	Forward	GCTCTATGGGAAGGACCAGC
	Reverse	TGGATCAGCAGCAAGTCCAG
HIF1A	Forward	ATGAGCTTGCTCATCAGTTGCC
	Reverse	TCACCAGCATCCAGAAGTTTCC

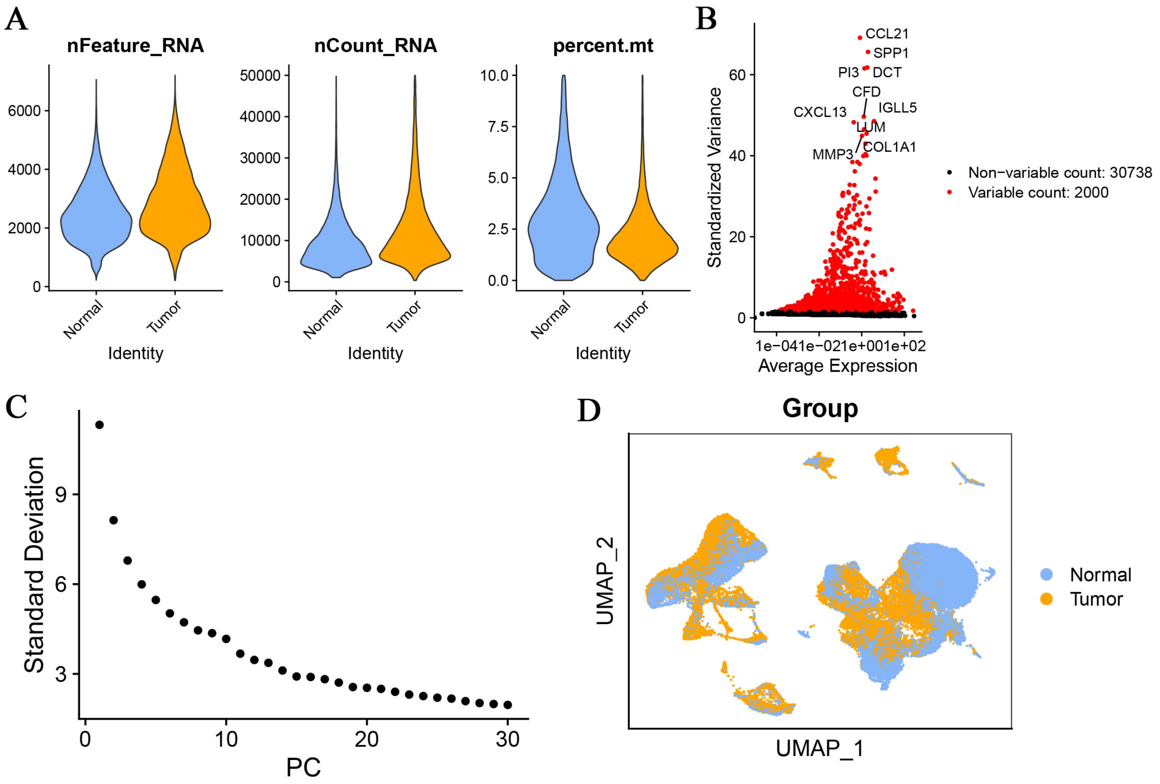

Figure S1 Quality control and preprocessing of single-cell RNA-seq data. (A) Filtering of low-quality cells based on standard QC metrics. (B) Identification of highly variable genes after normalization of the expression matrix. (C) Principal component analysis (PCA) and determination of the top 30 principal components using an elbow plot for downstream analyses. (D) Batch correction results showing no significant batch effects between experimental groups.

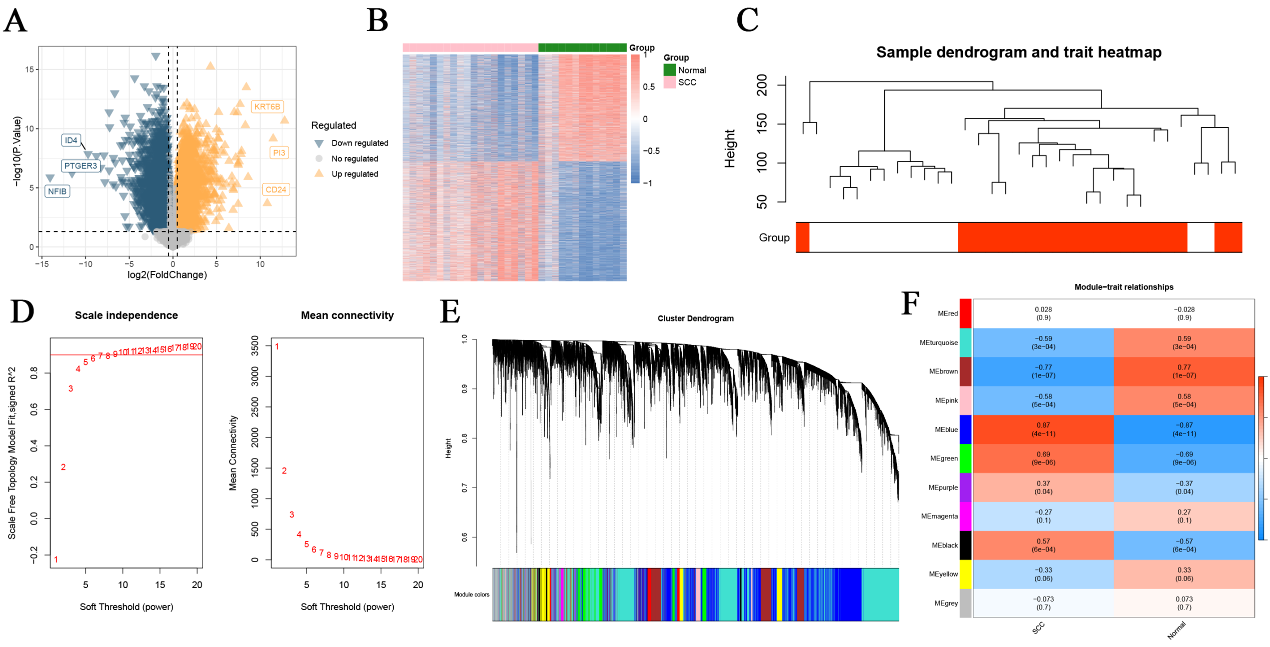

Figure S2 Identification of differentially expressed genes (DEGs) and WGCNA-derived key module genes. (A,B) Volcano plot and heatmap summarizing differential expression analysis in the training dataset. (C,D) Soft-threshold selection and network construction. (E) Hierarchical clustering dendrogram. (F) Module-trait relationships.

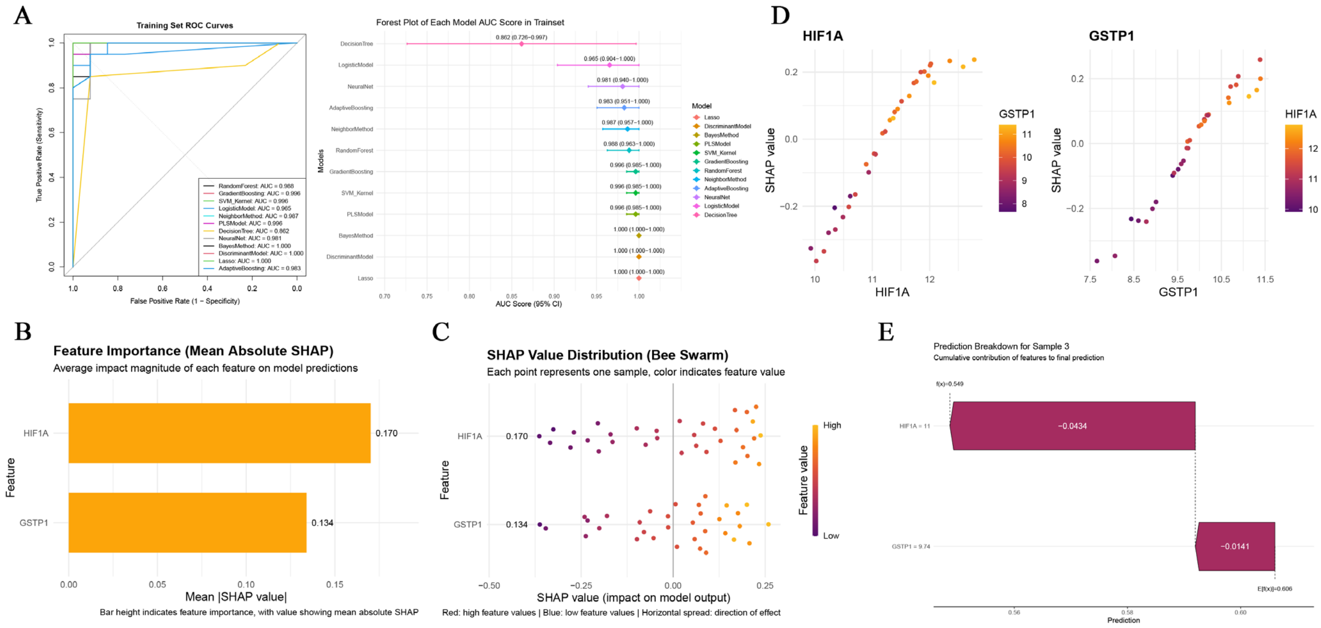

Figure S3 Diagnostic model construction and SHAP-based interpretability. (A) ROC curves comparing the diagnostic performance of ten machine learning models, with LASSO showing the highest AUC. (B,C) SHAP summary plots illustrating feature contributions of key genes HIF1A and GSTP1 to prediction accuracy. (D) Interaction effects between HIF1A and GSTP1 in disease prediction. (E) Feature importance ranking and predictive contribution of HIF1A and GSTP1 within the diagnostic model.

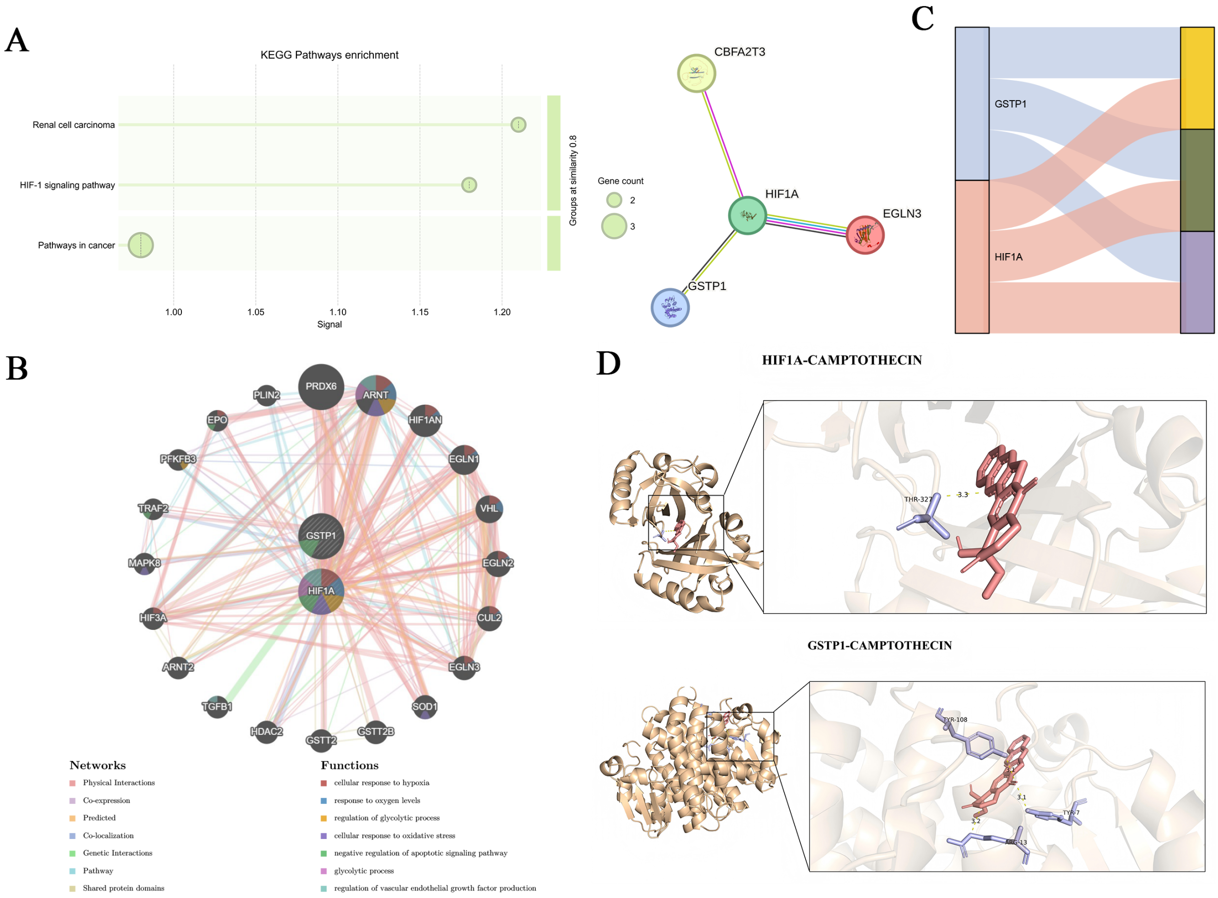

Figure S4 Protein-protein interaction (PPI) and gene-gene interaction (GGI) networks, drug prediction, and molecular docking. (A) PPI network showing 4 nodes and 3 edges. (B) GGI network of key genes. (C) Predicted drug compounds targeting key genes. (D) Molecular docking results demonstrating binding affinities between key genes and drugs.

Table S2 Molecular docking results

Drug	PubChem CID	Gene	PDB	Binding energy
Camptothecin	24360	HIF1A	4h6j	–8.7
Hydroquinone	785	HIF1A	4h6j	–5
Resveratrol	445154	HIF1A	4h6j	–7
Camptothecin	24360	GSTP1	2a2r	–8.6
Hydroquinone	785	GSTP1	2a2r	–5.1
Resveratrol	445154	GSTP1	2a2r	–6.8