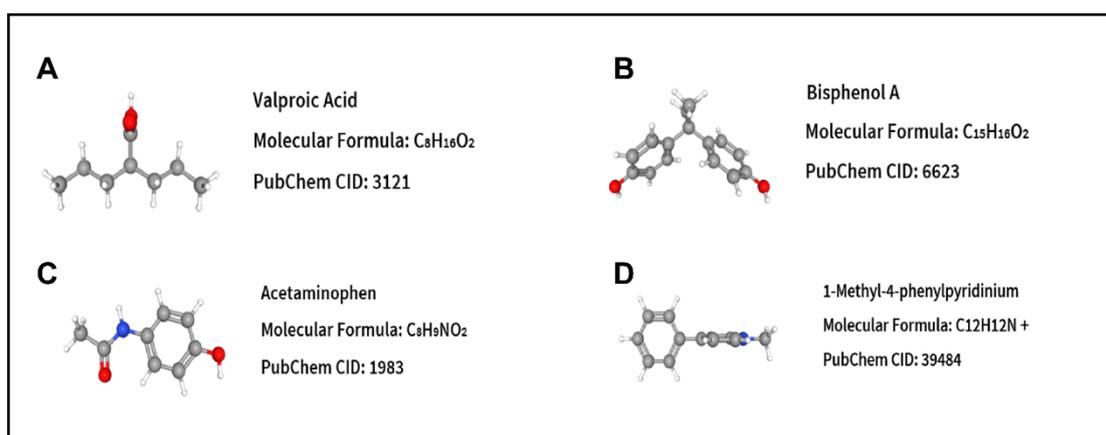**Supplementary Table 1 Baseline characteristics of the patients in the The Cancer Genome Atlas- Liver hepatocellular carcinoma cohort**

characteristics	TCGA-LIHC cohort
Number of patients	374
Gender (%)	
Female	121(32.4)
Male	253(67.6)
Age (median, range)	61(16-90)
Tumor grade (%)	
G1+G2	233(62.3)
G3+G4	136(36.4)
Unknown	5(1.3)
Stage (%)	
I+II	260(69.5)
III+IV	90(24.1)
Unknown	24(6.4)
AFP (%)	
≤400ng/ml	215(57.5)
＞400ng/ml	65(17.4)
Unknown	94(25.1)
Vascular Invasion (%)	
Yes	110(29.4)
No	208(55.6)
Unknown	56(15.0)
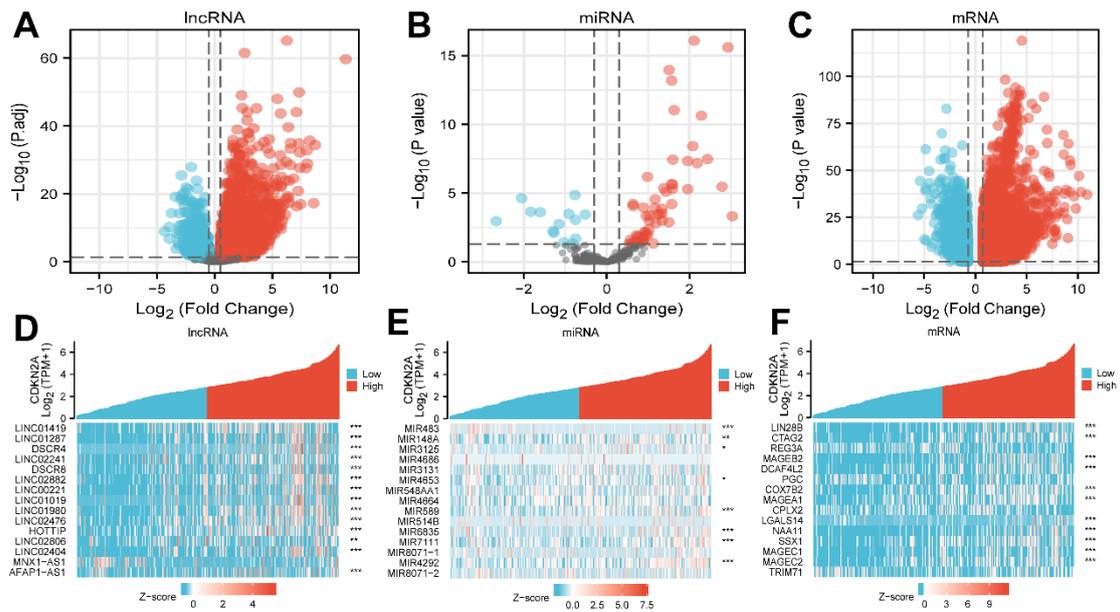
Supplementary Figure 1 Volcano plots and heatmap plots of differentially expressed long non-coding RNAs, differentially expressed microRNAs, and differentially expressed messenger RNAs between the expression of hepatocellular carcinoma samples and normal samples.

A–C: The volcano plots describe (A) 4544 differentially expressed long non-coding RNAs (|log2fold change| > 0.5 and adjusted *P* value < 0.05), (B) 69 differentially expressed microRNAs (|log2fold change| > 0.3 and adjusted *P* value < 0.05), and (C) 6560 differentially expressed messenger RNAs (|log2fold change| > 0.5 and adjusted *P* value < 0.05). D–F: The horizontal axis of the heatmap indicates the samples, and the vertical axis of the heatmap indicates 15 significant differentially expressed genes.

A Valproic Acid
Molecular Formula: $C_8H_{16}O_2$
PubChem CID: 3121

B Bisphenol A
Molecular Formula: $C_{15}H_{16}O_2$
PubChem CID: 6623

C Acetaminophen
Molecular Formula: $C_8H_9NO_2$
PubChem CID: 1983

D 1-Methyl-4-phenylpyridinium
Molecular Formula: C12H12N +
PubChem CID: 39484

Supplementary Figure 2 Prediction results of potential traditional Chinese medicine active components for the treatment of hepatocellular carcinoma based on growth arrest-specific 5.

(A–D) Prediction results of targeted traditional Chinese medicine active components.