molecules

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Supplementary Materials

Interpretation of *Euphorbia kansui* stir-fried with vinegar treating malignant ascites by a UHPLC-Q-TOF based rat serum and urine metabolomics strategy coupled with network analysis

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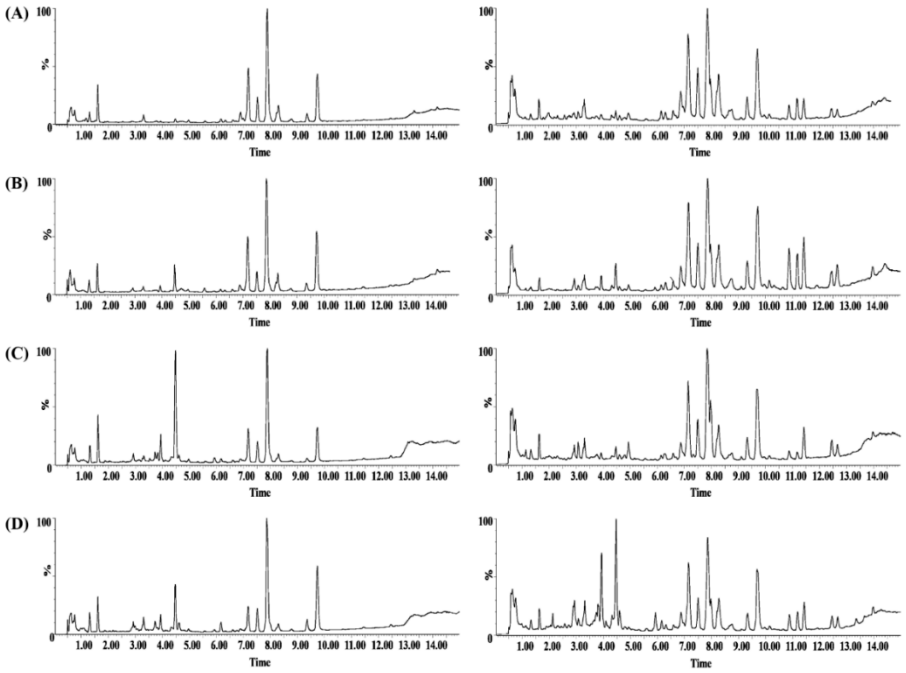

Figure S1. The representative base peak intensity chromatograms of serum samples (A-D) from four groups by UPLC-Q-TOF in positive (Left) and negative (Right) modes. A-D represent the Control, Model, Kansui, and V-kansui groups, respectively.

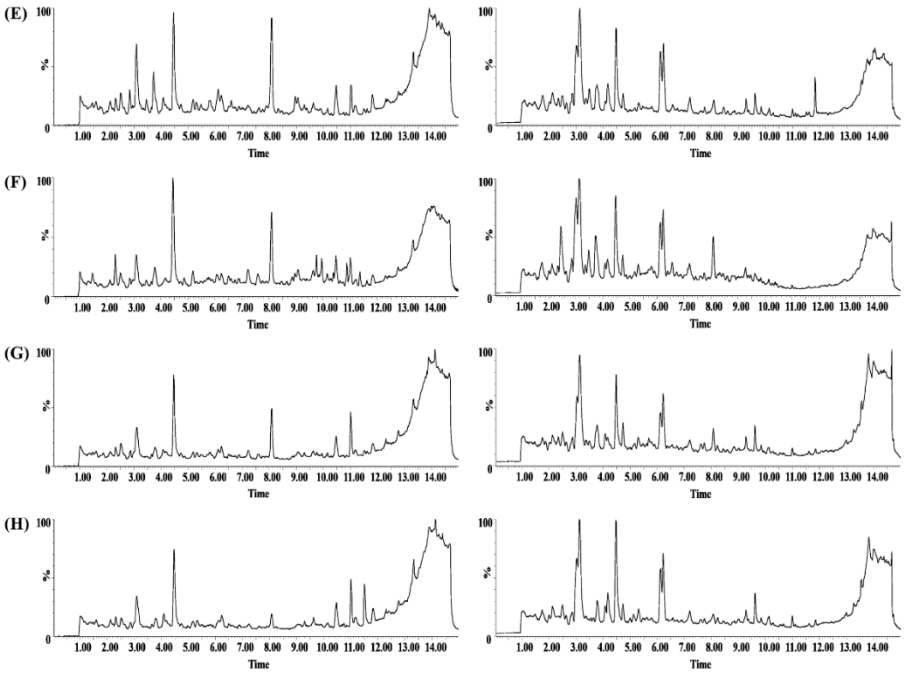

Figure S2. Representative base peak intensity chromatograms of urinary samples (E-H) of four groups by UHPLC-Q-TOF in positive (Left) and negative (Right) modes. E-H represent the Control, Model, Kansui, and V-kansui groups, respectively.

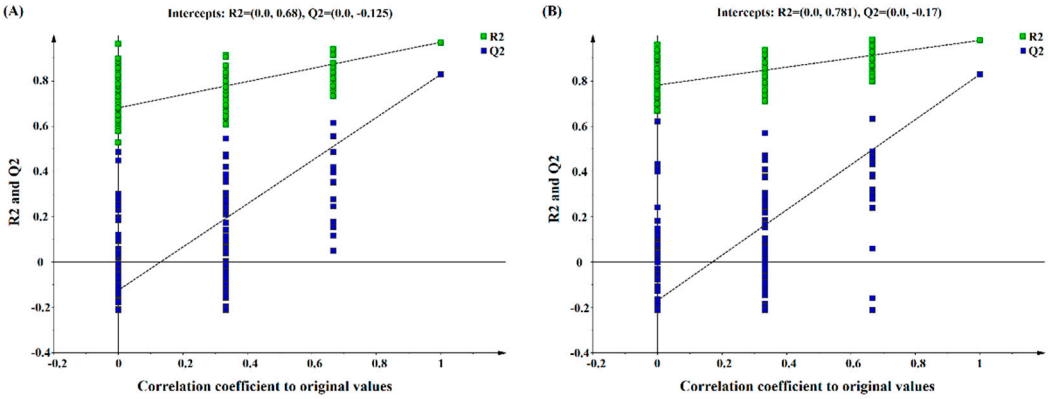

Figure S3. The response permutation test plots (*n*=200) for the OPLS-DA models for serum (A) and urine samples (B) in positive mode.

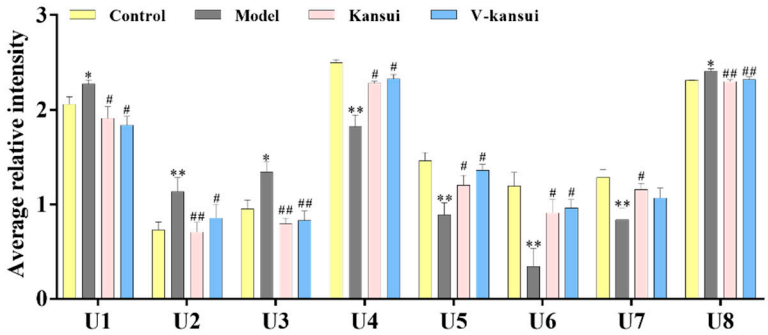

Figure S4. The average relative intensity changes of urine endogenous metabolites from different groups. Comparing the model group with the control group, * indicates $p < 0.05$, and ** indicates $p < 0.01$.; Comparing

the kansui group and V-kansui group with the model group, # indicates $p < 0.05$, and ## indicates $p < 0.01$indicates $p < 0.05$.

Table S1. UPLC-Q-TOF-MS data for Identification results of potential biomarkers

Metabolites	RT	Adduct	*m/z*	Mass error (ppm)	Fragments	Databases/Literatures
Indoleacetaldehyde	1.18	M+H	160.0698	8.7	145, 117	METLIN
Taurocholic acid	2.88	M-H	514.2942	5.0	124	METLIN
Taurochenodesoxycholic acid	3.91	M-H	498.2991	4.8	480, 462, 372, 124, 80	HMDB
Cholic acid	4.46	M-H	407.2886	2.4	343, 289	METLIN
Phytosphingosine	4.79	M+H	318.2912	-5.3	301, 300, 282, 197	METLIN, HMDB
Chenodeoxycholic acid	6.15	M-H	391.2934	2.0	373, 345, 268, 185	MASSBANK
LysoPC(18:1)	8.27	M+H	522.3438	-8.2	504, 283, 265, 241, 184, 166, 104	HMDB, METIN, [1,2]
Docosahexaenoic acid	10.88	M-H	327.2400	-0.6	283, 229	METLIN
5-Hydroxy-6-methoxyindole glucuronide/6-Hydroxy-5-methoxyindole glucuronide	3.73	M+H	340.0978	7.1	322, 164, 146, 132	HMDB, METLIN, [3]
Prostaglandin G_2	6.46	M+FA-H	413.2165	-9.0	287, 235, 113	METLIN, HMDB
10-Formyltetrahydrofolate	6.71	M-H	472.1692	7.0	455, 428, 293	HMDB
5-*L*-Glutamyl-taurine	7.22	M+H	255.0563	-3.5	237, 209, 194, 135, 126, 109	HMDB, METLIN, [4,5]
Riboflavin	8.96	M+H	377.1403	5.6	294, 243, 158	METLIN
Androstenedione	9.07	M+FA-H	331.1939	2.1	285, 267, 269	HMDB
11b-Hydroxyprogesterone	9.64	M-H	331.1973	-4.2	313, 287	HMDB
Phytosphingosine	10.48	M+H	318.2924	-1.6	300, 301, 282, 197	METLIN, HMDB

References:

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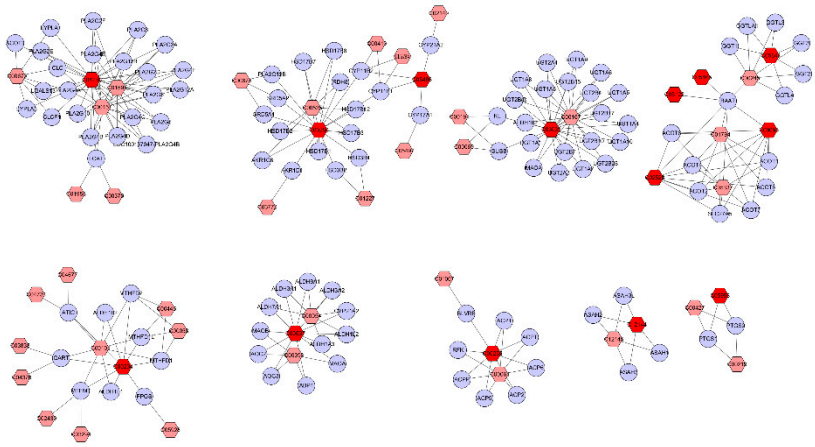

Figure S5. The network of potential metabolites for pathway-based genes. The red nodes represent the potential metabolites and grey nodes represent the related genes.

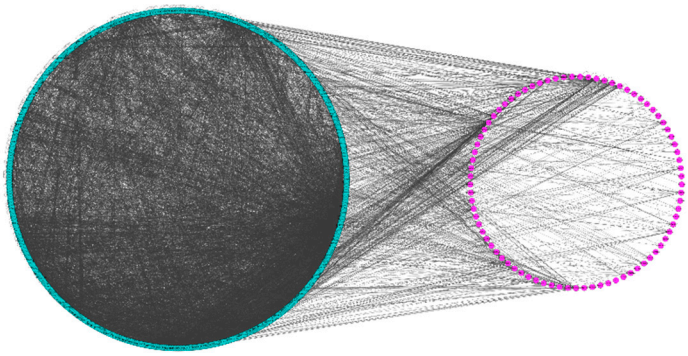

Figure S6. The extended protein-protein network of metabolites-related genes. The blue and pink nodes represent adjacent proteins and metabolite-related proteins, respectively.

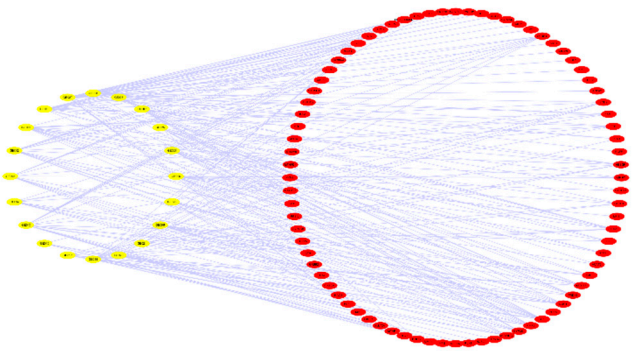

Figure S7. The compound-target network representing the effect of treating malignant ascites by V-kansui. The yellow and red nodes represent compounds and disease-related proteins, respectively.

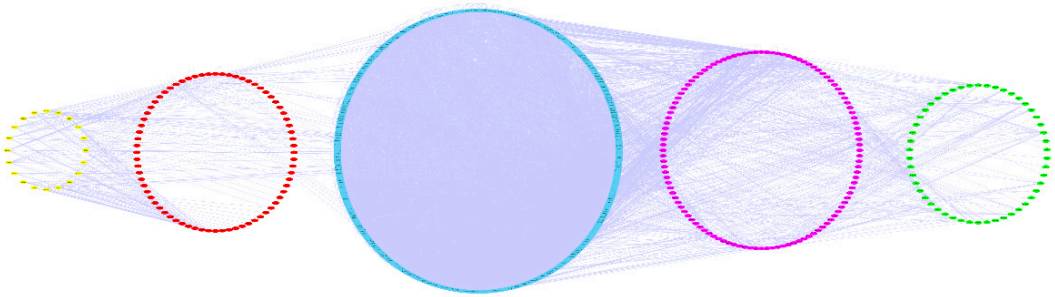

Figure S8. The compound-target-metabolite network. The yellow, red, blue, pink and green nodes represent the active compounds, targets, adjacent proteins, pathway genes and potential metabolites, respectively.

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