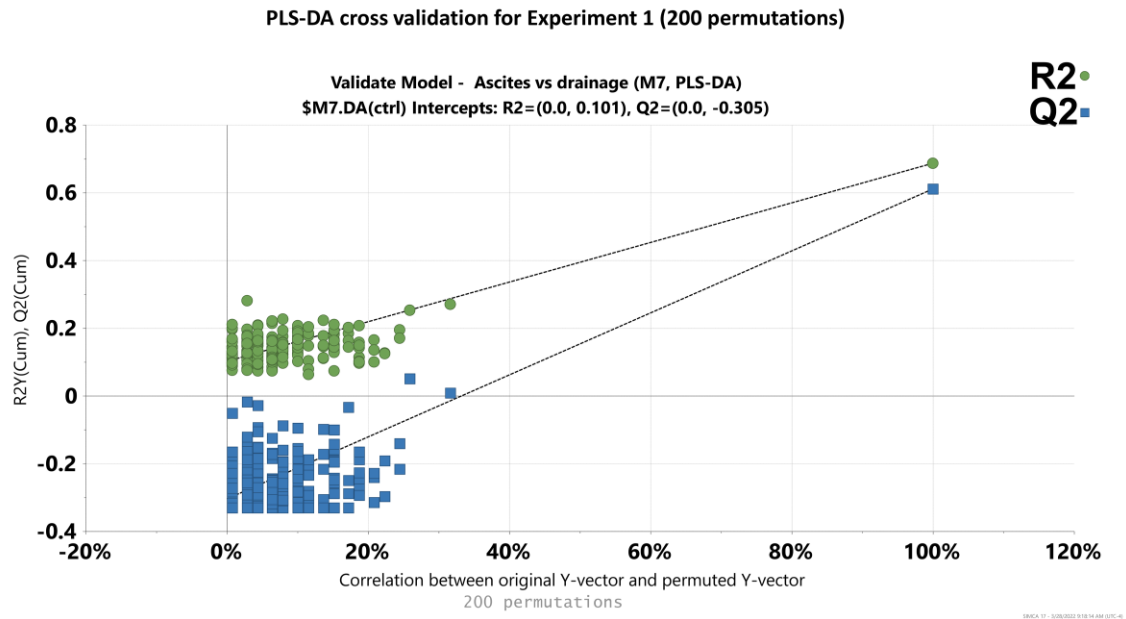


Figure S1. PCA Variances and scores plots for Experiment 1

A, magnitude of variances; **B**, PCA scores plot principal component 1 (PC1) vs. principal component 2 (PC2) showing 95% confidence ellipses; **C**, PCA scores plot principal component 1 (PC1) vs. principal component 3 (PC3) showing 95% confidence ellipses; **D**, PCA scores plot principal component 2 (PC2) vs. principal component 3 (PC3) showing 95% confidence ellipses. Red ellipse and scores represent cirrhotic ascites patient ascites fluid. Green ellipse and scores represent drainage fluid from control postoperative surgical patients.

A



B

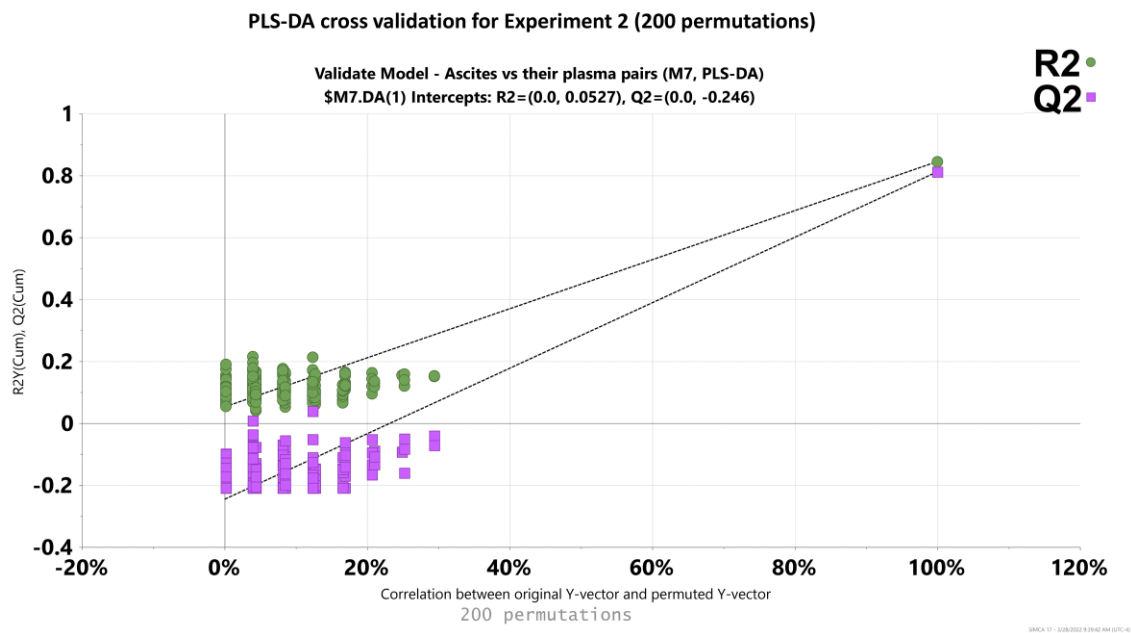


Figure S2. Leave-one-out cross validation of the PLS-DA models for Experiment 1 (A) and Experiment 2 (B)

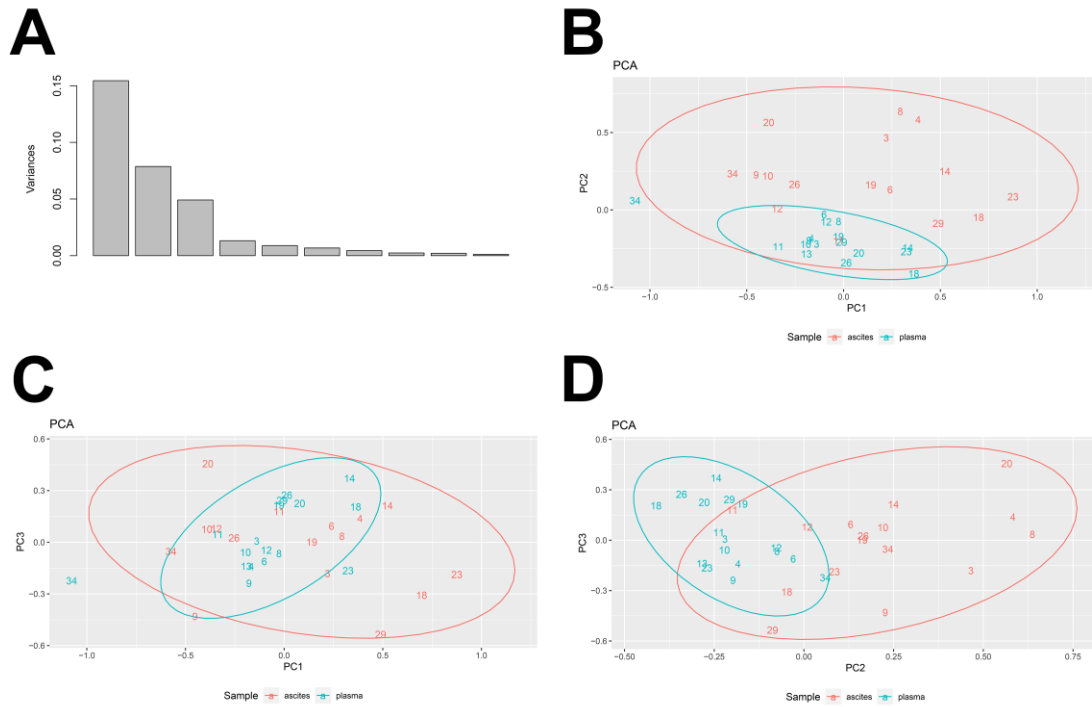
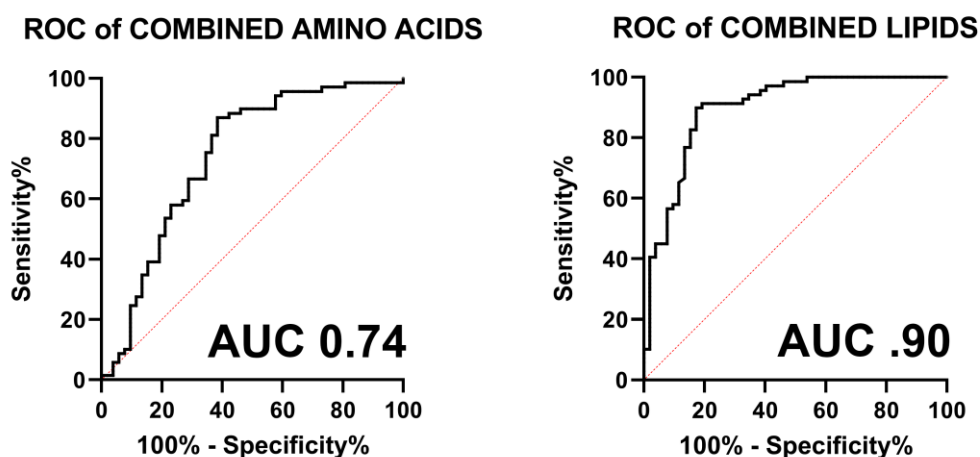


Figure S3. PCA Variances and scores plots for Experiment 2

A, magnitude of variances; **B**, PCA scores plot principal component 1 (PC1) vs. principal component 2 (PC2) showing 95% confidence ellipses; **C**, PCA scores plot principal component 1 (PC1) vs. principal component 3 (PC3) showing 95% confidence ellipses; **D**, PCA scores plot principal component 2 (PC2) vs. principal component 3 (PC3) showing 95% confidence ellipses. Red ellipse and scores represent cirrhotic ascites patient ascites fluid. Green ellipse and scores represent cirrhotic ascites patient plasmas.

A. Experiment 1



B. Experiment 2

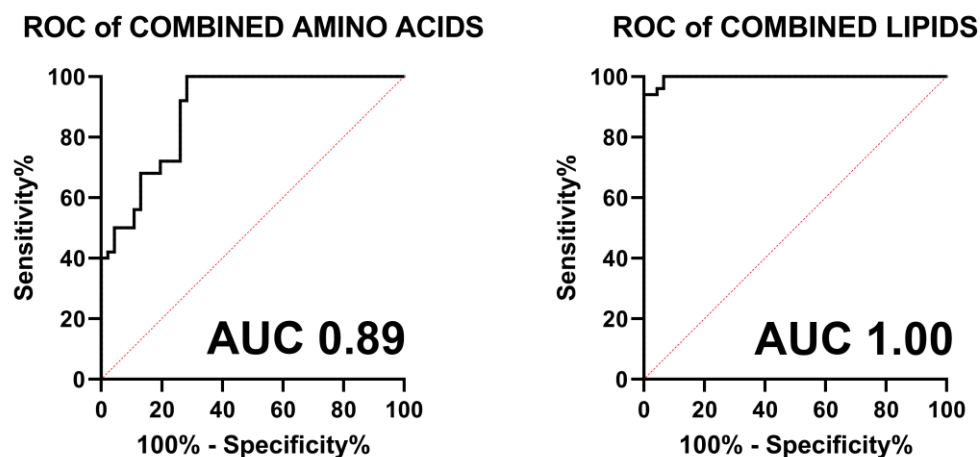


Figure S4. ROC analysis for **A.** combined elevated amino acids and combined diminished lipids in ascites fluid for Experiment 1 and **B.** combined elevated amino acids and combined diminished lipids in ascites fluid for Experiment 2

All ROC analyses were significant ($P < 0.0001$).

Experiment 1. Combined elevated amino acids were glutamine, proline, histidine and tyrosine. Combined diminished lipids were lauric, myristic, palmitic, linoleic, oleic and stearic acids, together with cholesterol (Table 1).

Experiment 2. Combined elevated amino acids were glycine, valine, proline, threonine, methionine, lysine, glutamine, phenylalanine and tyrosine. Combined diminished lipids were myristic, palmitic, oleic, vaccenic and stearic acids, together with cholesterol (Table 2).

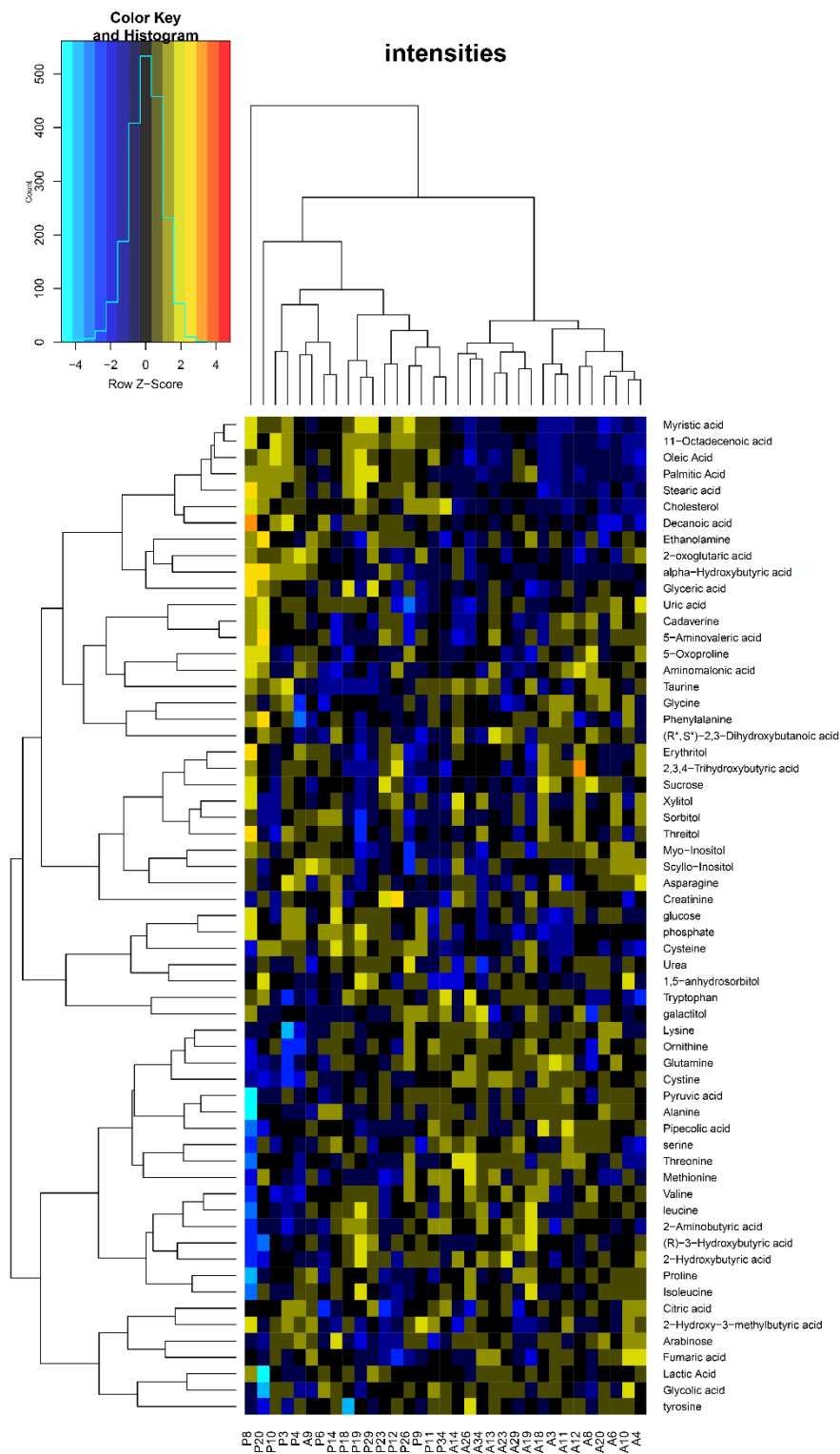


Figure S5. Heatmap showing all ascites and plasma samples from Experiment 2 and all metabolite features.

Table S1. Metabolites detected by GC-MS in ascitic fluid and plasma from ascites patients and peritoneal fluid from postoperative surgical patients

Metabolite	Retention time (min)	Derivatives formed
Ethanolamine	9.25	2TMS
Propylene glycol	9.33	2TMS
Pyruvic acid	9.59	1TMS
Lactic acid	9.79	2TMS
Glycolic acid	9.98	2TMS
Alanine	10.43	2TMS
Glycine	10.67;13.53	2TMS; 3TMS
2-Hydroxybutyric acid	10.82	2TMS
3-Hydroxybutyric acid	11.30	2TMS
2-Hydroxy-3-methylbutyric acid	11.41	2TMS
2-Aminobutyric acid	11.55	2TMS
Urea	11.70;12.51;12.63	2TMS; 3TMS
2-Ketoisocaproic acid	12.12	1TMS; 1MOX
Valine	12.19	2TMS
Leucine	13.00	2TMS
Phosphate	13.10	3TMS
Isoleucine	13.32	2TMS
Proline	11.59; 13.41	1TMS; 2TMS
Glyceric acid	13.83	3TMS
Fumaric acid	13.94	2TMS
2,3-Dihydroxybutanoic acid	14.18	3TMS
Serine	14.24	3TMS
Uracil	14.31	2TMS
Pipecolic acid	14.35	2TMS
Threonine	14.62	3TMS
Cadaverine	15.08	3TMS
Aminomalonic acid	15.73	3TMS
4-Chlorophenylacetic acid (ISTD)	15.90	1TMS
Erythritol	16.21	4TMS
Methionine	16.35	2TMS
5-Oxoproline	16.40	2TMS
2,3,4-Trihydroxybutyric acid	16.66	4TMS
Cysteine	16.79	3TMS
Creatinine	16.88	3TMS
2-Oxoglutaric acid	16.96	2TMS; 1MOX
5-Aminovaleric acid	17.34	3TMS
Ornithine	17.45	3TMS
Glutamic acid	17.50	3TMS
Phenylalanine	17.68	2TMS
Lauric acid	17.78	1TMS
Asparagine	18.13	3TMS
Taurine	18.20	3TMS
Lysine	18.50; 20.84	3TMS; 4TMS
Xylitol	18.79	5TMS
Galactitol	18.84	6TMS
Glutamine	19.26	3TMS
Threitol	19.40	4TMS
Citric acid	19.81	4TMS
Myristic acid	19.92	1TMS
1,5-Anhydrosorbitol	20.19	4TMS
Arabinose	20.28	5TMS; 1MOX
Fructose	20.47; 20.55	5TMS; 1MOX 5TMS; 1MOX
Galactose	20.62	5TMS; 1MOX

Glucose	20.66; 20.76	5TMS; 1MOX 5TMS; 1MOX
Histidine	20.88	3TMS
Tyrosine	21.03	3TMS
Mannitol	21.09	5TMS; 1MOX
Mannose	21.44	5TMS
Gluconic acid	21.82	6TMS
Palmitic acid	21.87	1TMS
Scyllo-inositol	22.05	6TMS
Uric acid	22.62	4TMS
Myo-inositol	22.65	6TMS
Sorbitol	22.86	6TMS
Linoleic acid	23.42	1TMS
Oleic acid	23.46	1TMS
Vaccenic acid	23.51	1TMS
Stearic acid	23.65	1TMS
Tryptophan	23.73	3TMS
Sucrose	27.38	8TMS
Cholesterol	33.57	1TMS