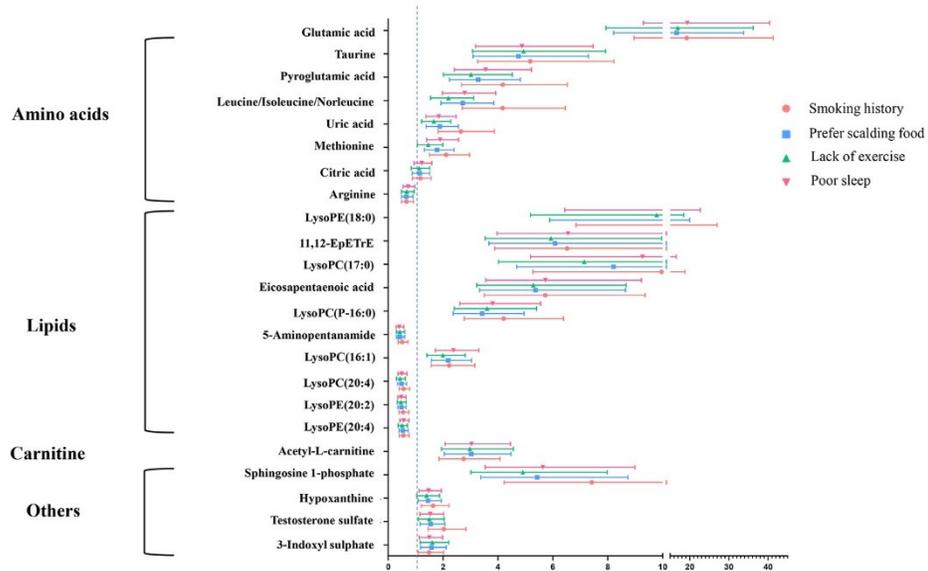
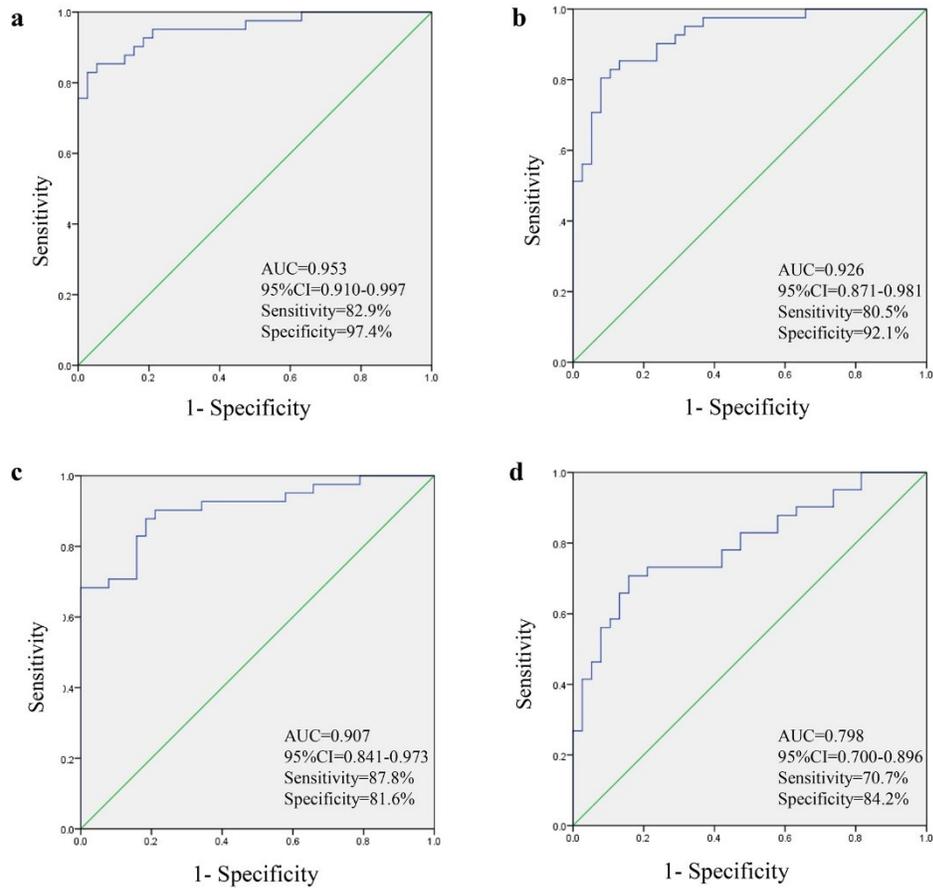


Supplementary Material

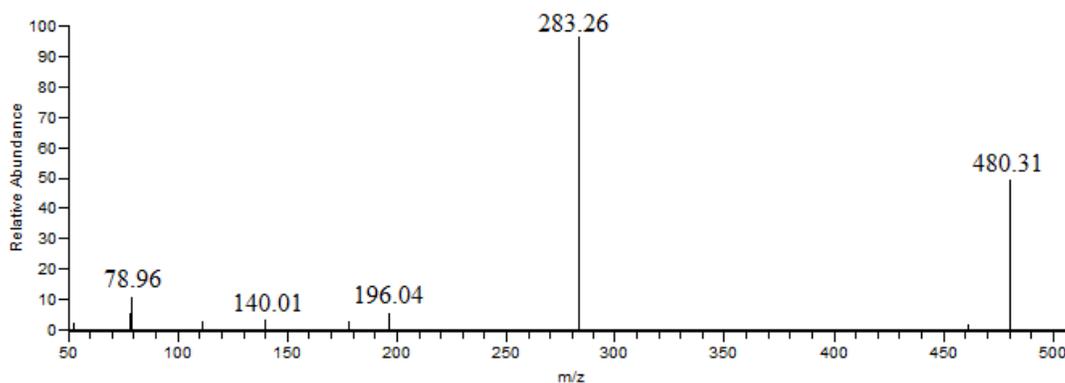


Supplementary Figure S1 ORs per SD increment (95% CI) of each metabolite based on results from multivariate-adjusted conditional logistic regression models.

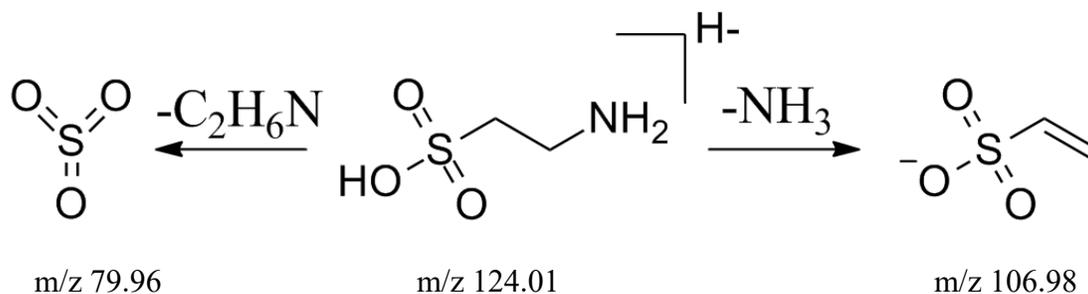


Supplementary Figure S2 The ROC curve with AUC, CI, sensitivity, specificity of (a) Diagnosis panel in training set, (b) Glutamic acid, (c) LysoPE(18:0) and (d) Taurine, respectively. AUC: Area under curve; CI: Confidence interval.

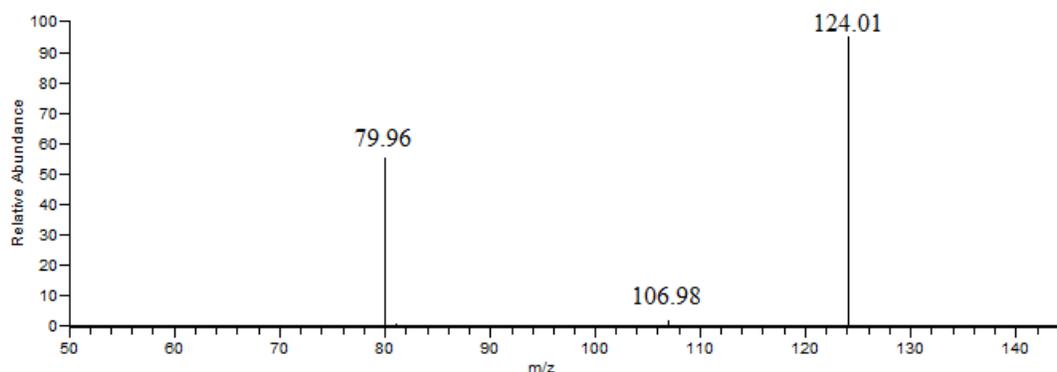
QC-N-400-1200 #1803 RT: 9.59 AV: 1 NL: 1.16E5
 F: FTMS - p ESI d Full ms2 480.3090@hcd40.00 [50.0000-510.0000]



c



QC-N-80-180 #321 RT: 1.03 AV: 1 NL: 5.11E5
 F: FTMS - p ESI d Full ms2 124.0070@hcd40.00 [50.0000-145.0000]



Supplementary Figure S3 The structures of three metabolic biomarkers and the mass fragmentation pathways. (a) Glutamic acid ($\text{C}_5\text{H}_9\text{NO}_4$) was observed under negative mode (m/z 146.05), and the fragment ions were 128.04 $[\text{M}-\text{H}-\text{H}_2\text{O}]^-$, 102.06 $[\text{M}-\text{H}-\text{CO}_2]^-$ and 85.03 $[\text{M}-\text{H}-\text{CO}_2-\text{NH}_3]^-$; (b) LysoPE(18:0) ($\text{C}_{23}\text{H}_{48}\text{NO}_7\text{P}$) was observed under negative mode (m/z 480.31), and the fragment ions were 283.26 $[\text{M}-\text{H}-\text{C}_5\text{H}_{12}\text{O}_5\text{NP}]^-$, 196.04 $[\text{M}-\text{H}-\text{C}_{18}\text{H}_{36}\text{O}_2]^-$, 140.01 $[\text{M}-\text{H}-\text{C}_{18}\text{H}_{36}\text{O}_2-\text{C}_3\text{H}_4\text{O}]^-$, 78.96 $[\text{M}-\text{H}-\text{C}_{18}\text{H}_{36}\text{O}_2-\text{C}_3\text{H}_4\text{O}-\text{C}_2\text{H}_7\text{ON}]^-$; (c) Taurine ($\text{C}_2\text{H}_7\text{NO}_3\text{S}$) was observed under negative mode (m/z 124.01), and the fragment ions were 106.98 $[\text{M}-\text{H}-\text{NH}_3]^-$, 79.96 $[\text{M}-\text{H}-\text{C}_2\text{H}_6\text{N}]^-$.