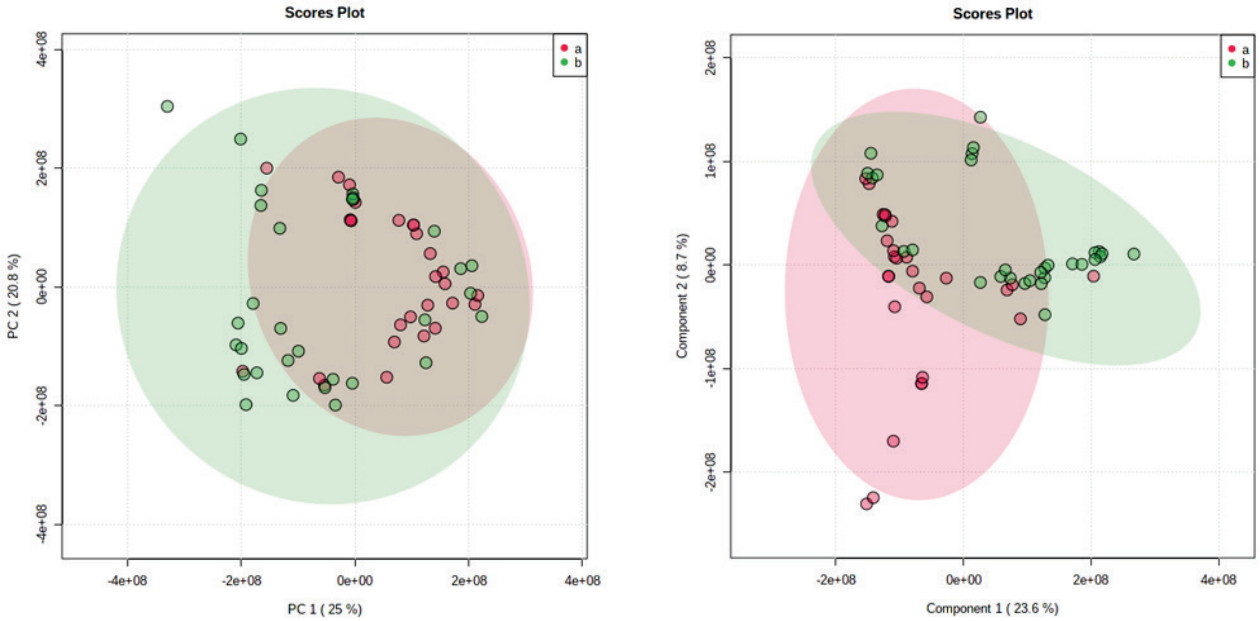
Supplementary material

We performed PCA and PLS-DA analyzes based on NMR spectra binned to bins of 0.001 ppm. We left out water region 4.6-5.0 ppm, and used NMR spectra from 0.5 ppm to 9.0 ppm. The result of PCA and PLS-DA analyzes are shown on Supplementary Figure 1.



Supplementary Fig. 1. PCA (left) and PLS-DA (right) analyzes based on NMR spectral bins of 0.001 ppm, (**a**) AMI patients, (**b**) controls, performed online using Metaboanalyst 4.0. To show the reliability of PLS-DA method, we used leave-one-out cross-validation (LOOCV) and permutation test. The validation results are summarized in Table S1. The permutation test performed with $p<0.01$ (0/100).

Supplementary Table 1. Details from LOOCV PLS-DA validation.

Measure	**1 comps**	**2 comps**	**3 comps**	**4 comps**	**5 comps**	**6 comps**	**7 comps**	**8 comps**
Accuracy	0.76271	0.77966	0.77966	0.79661	0.79661	0.77966	0.79661	0.77966
R2	0.30297	0.44752	0.4922	0.53222	0.56052	0.58769	0.62336	0.65369
Q2	0.16529	0.25991	0.29227	0.30281	0.28668	0.28188	0.27459	0.23037