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SUPPLEMENTAL DATA

Serum amino acid profiles in acute myocardial infarction: NMR metabolomics comparison of STEMI, NSTEMI, and controls

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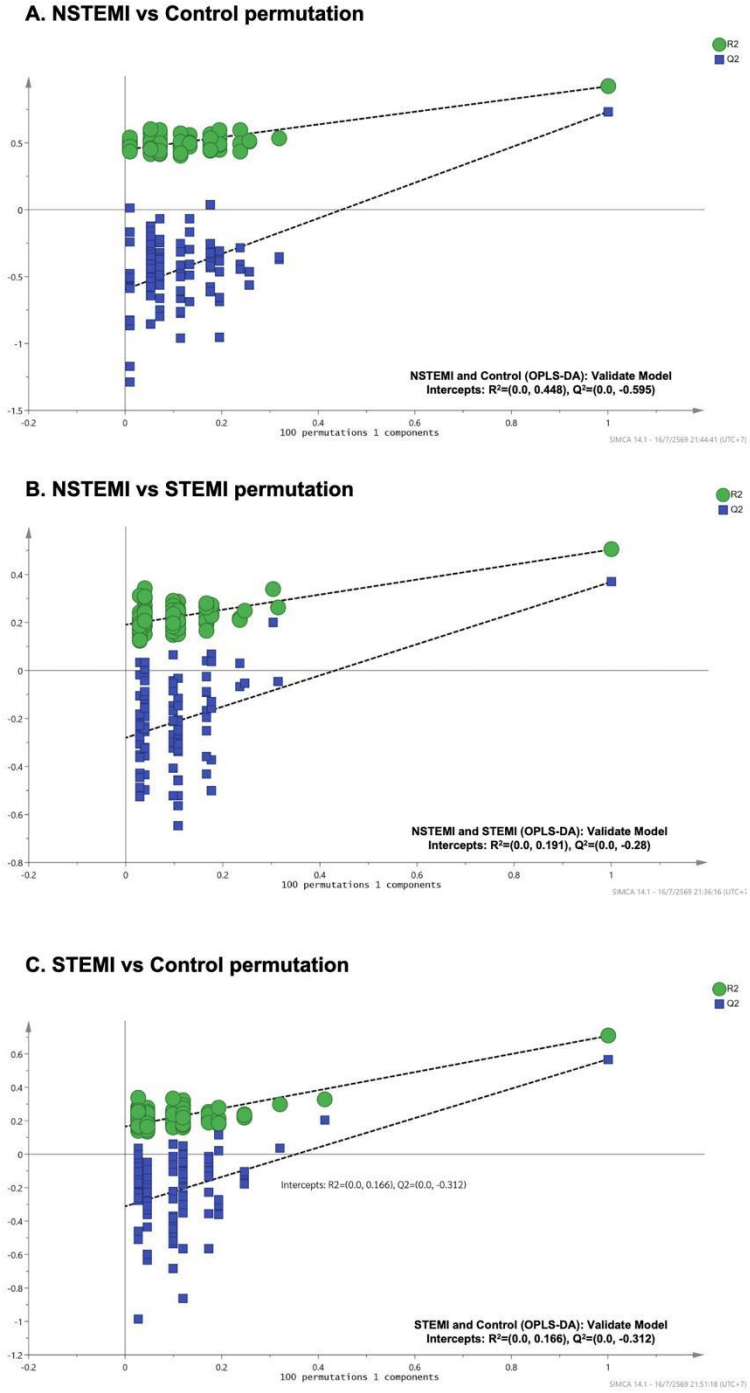


Figure S1. Permutation testing of the OPLS-DA models for pairwise group comparisons. Permutation tests based on 100 random permutations were performed for **(A)** NSTEMI versus control, **(B)** NSTEMI versus STEMI, and **(C)** STEMI versus control. Green circles represent R^2 values, blue squares represent Q^2 values, and the points at a correlation coefficient of 1 correspond to the original models. Dashed lines indicate the regression lines derived from the permuted models. The Q^2 intercepts

were −0.595, −0.280, and −0.312 for the NSTEMI versus control, NSTEMI versus STEMI, and STEMI versus control comparisons, respectively. The negative Q^2 intercepts and the superior R^2 and Q^2 values of the original models relative to the permuted models support model robustness and indicate no evidence of substantial overfitting. **Abbreviations:** NSTEMI, non-ST-segment elevation myocardial infarction; OPLS-DA, orthogonal projections to latent structures discriminant analysis; Q^2, cross-validated predictive ability; R^2, explained variance; STEMI, ST-segment elevation myocardial infarction.

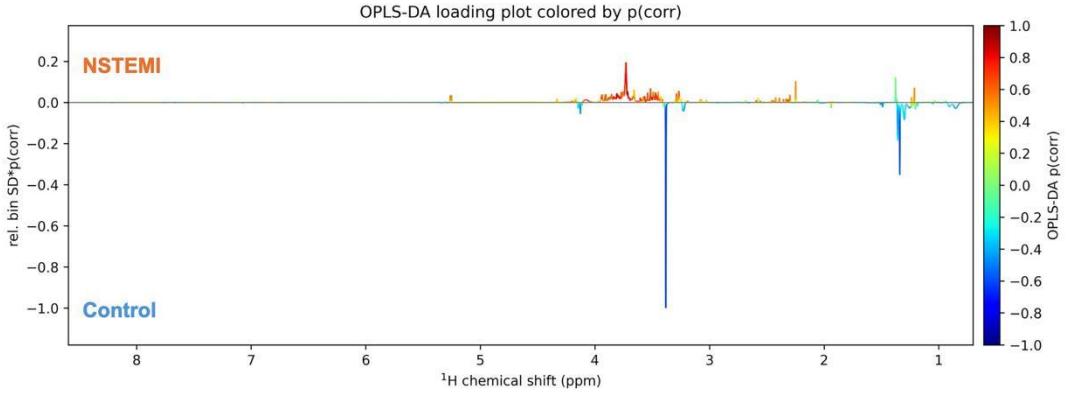


Figure S2. OPLS-DA loading plot for the comparison between the NSTEMI and control groups. The loading plot is colored according to p(corr), showing the contribution and direction of individual spectral variables to group discrimination. The x-axis represents the ^{1}H NMR chemical shift in ppm, whereas the y-axis represents the scaled loading value calculated as the relative bin SD multiplied by p(corr). Positive p(corr) values, shown in yellow to red, indicate spectral variables associated with the NSTEMI group, whereas negative values, shown in cyan to blue, indicate variables associated with the control group. Variables with larger absolute p(corr) values contributed more strongly to separation between the groups. **Abbreviations:** NMR, nuclear magnetic resonance; NSTEMI, non-ST-segment elevation myocardial infarction; OPLS-DA, orthogonal projections to latent structures discriminant analysis; p(corr), correlation-scaled loading; ppm, parts per million; SD, standard deviation.

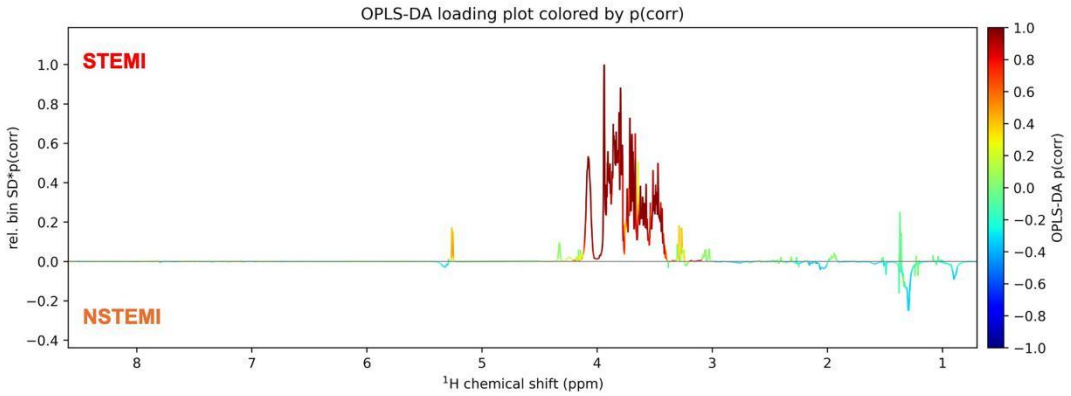


Figure S3. OPLS-DA loading plot for the comparison between the STEMI and NSTEMI groups. The loading plot is colored according to p(corr), illustrating the direction and contribution of individual spectral variables to group discrimination. The x-axis represents the ^{1}H NMR chemical shift in ppm, whereas the y-axis represents the scaled loading value calculated as the relative bin SD multiplied by p(corr). Positive p(corr) values, displayed in yellow to red, indicate spectral variables associated with STEMI, while negative values, displayed in cyan to blue, indicate variables associated with NSTEMI. Variables with larger absolute p(corr) values contributed more strongly to the separation between the groups. **Abbreviations:** NMR, nuclear magnetic resonance; NSTEMI, non-ST-segment elevation myocardial infarction; OPLS-DA, orthogonal projections to latent structures discriminant analysis; p(corr), correlation-scaled loading; ppm, parts per million; SD, standard deviation; STEMI, ST-segment elevation myocardial infarction.

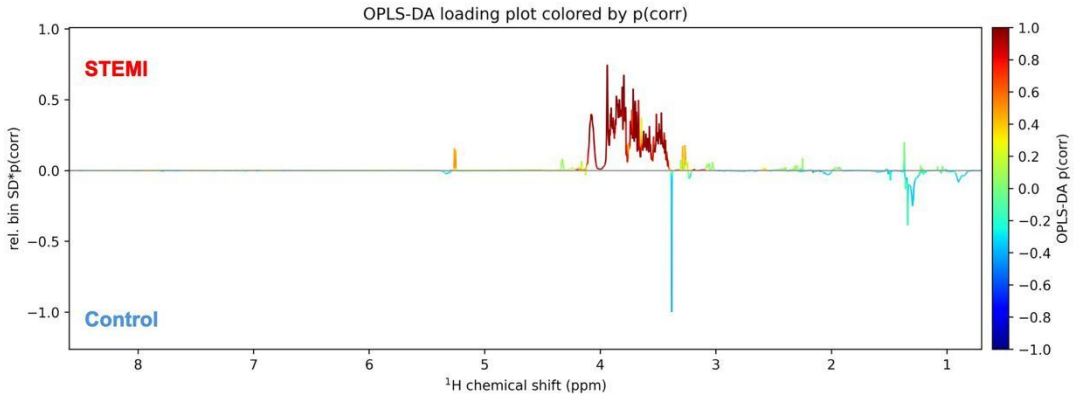


Figure S4. OPLS-DA loading plot for the comparison between the STEMI and control groups. The loading plot is colored according to p(corr), illustrating the direction and contribution of individual NMR spectral variables to group discrimination. The x-axis represents the ^{1}H chemical shift in ppm, whereas the y-axis represents the scaled loading value calculated as the relative bin SD multiplied by p(corr). Positive p(corr) values, displayed in yellow to red, indicate spectral variables associated with STEMI, whereas negative values, displayed in cyan to blue, indicate variables associated with the control group. Variables with larger absolute p(corr) values contributed more strongly to the separation between the groups. **Abbreviations:** NMR, nuclear magnetic resonance; OPLS-DA, orthogonal projections to latent structures discriminant analysis; p(corr), correlation-scaled loading; ppm, parts per million; SD, standard deviation; STEMI, ST-segment elevation myocardial infarction.

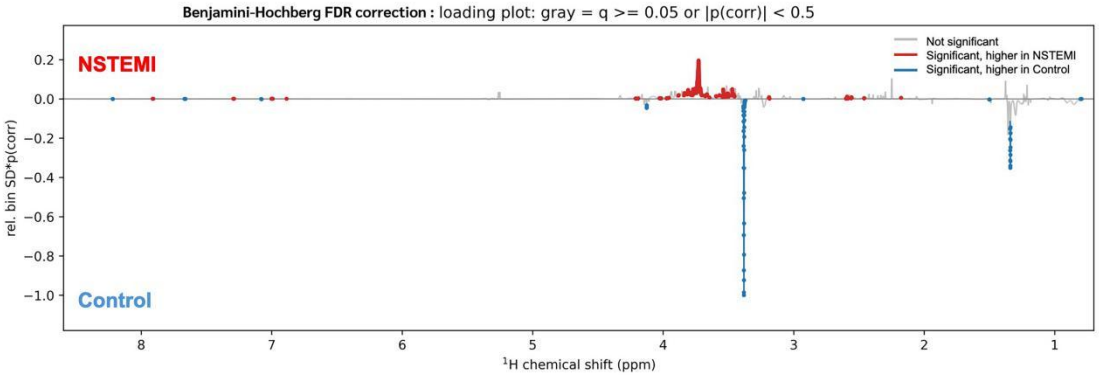


Figure S5. BH-FDR-corrected OPLS-DA coefficient loading plot for the comparison between the NSTEMI and control groups. Each vertical signal represents an individual ^{1}H NMR spectral bin, with the chemical shift shown on the x-axis and the scaled loading value, calculated as the relative bin SD multiplied by p(corr), shown on the y-axis. Spectral variables were considered significant when they met both criteria of $q < 0.05$ after BH-FDR correction and $|p(corr)| \geq 0.5$. Red signals indicate variables with higher relative abundance in the NSTEMI group, whereas blue signals indicate variables with higher relative abundance in the control group. Gray signals did not meet one or both significance criteria. **Abbreviations:** BH-FDR, Benjamini–Hochberg false discovery rate; NMR, nuclear magnetic resonance; NSTEMI, non-ST-segment elevation myocardial infarction; OPLS-DA, orthogonal projections to latent structures discriminant analysis; p(corr), correlation-scaled loading; SD, standard deviation.

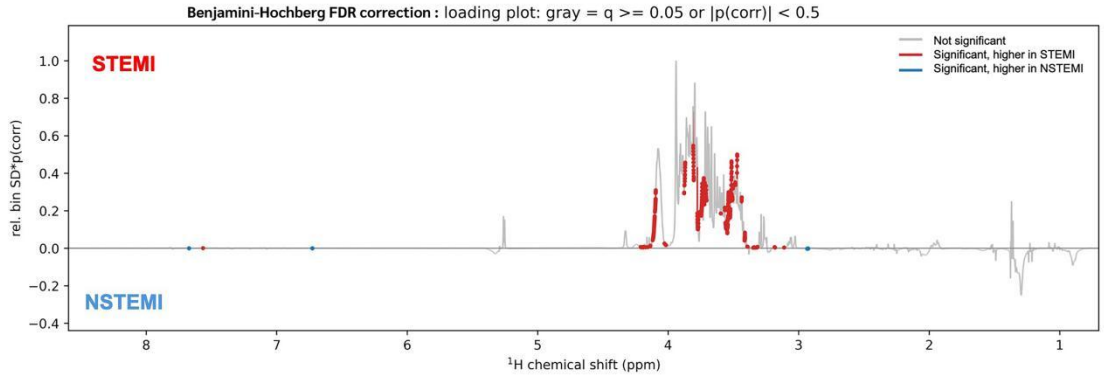


Figure S6. BH-FDR-corrected OPLS-DA coefficient loading plot for the comparison between the STEMI and NSTEMI groups. Each vertical signal represents an individual ^{1}H NMR spectral bin, with the chemical shift shown on the x-axis and the scaled loading value, calculated as the relative bin SD multiplied by p(corr), shown on the y-axis. Spectral variables were considered significant when they met both criteria of $q < 0.05$ after BH-FDR correction and $|p(corr)| \geq 0.5$. Red signals indicate variables associated with higher relative abundance in the STEMI group, whereas blue signals indicate variables associated with higher relative abundance in the NSTEMI group. Gray signals did not meet one or both significance criteria. **Abbreviations:** BH-FDR, Benjamini–Hochberg false discovery rate; NMR, nuclear magnetic resonance; NSTEMI, non-ST-segment elevation myocardial infarction; OPLS-DA, orthogonal projections to latent structures discriminant analysis; p(corr), correlation-scaled loading; SD, standard deviation; STEMI, ST-segment elevation myocardial infarction.

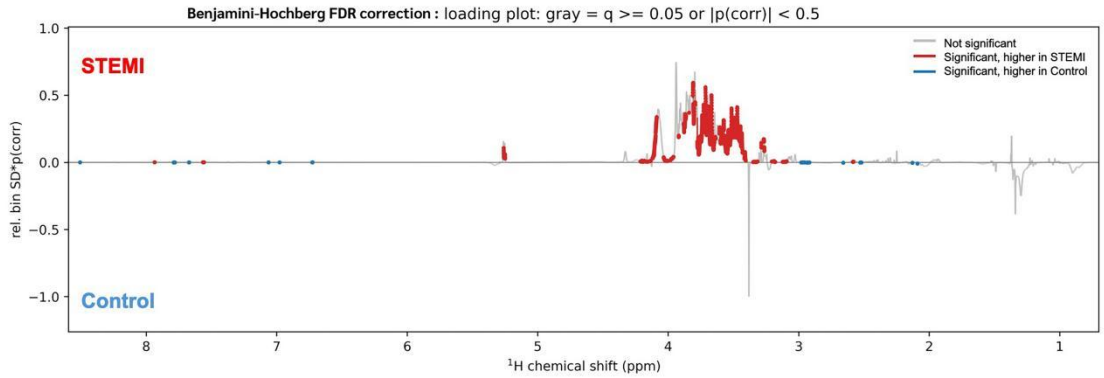


Figure S7. BH-FDR-corrected OPLS-DA coefficient loading plot for the comparison between the STEMI and control groups. Each vertical signal represents an individual ^{1}H NMR spectral bin, with the chemical shift shown on the x-axis and the scaled loading value, calculated as the relative bin SD multiplied by p(corr), shown on the y-axis. Spectral variables were highlighted only when they met both criteria of $q < 0.05$ after BH-FDR correction and $|p(corr)| \geq 0.5$. Red signals indicate variables associated with higher relative abundance in the STEMI group, whereas blue signals indicate variables associated with higher relative abundance in the control group. Gray signals did not meet one or both significance criteria. **Abbreviations:** BH-FDR, Benjamini–Hochberg false discovery rate; NMR, nuclear magnetic resonance; OPLS-DA, orthogonal projections to latent structures discriminant analysis; p(corr), correlation-scaled loading; ppm, parts per million; q, false discovery rate-adjusted p value; SD, standard deviation; STEMI, ST-segment elevation myocardial infarction.

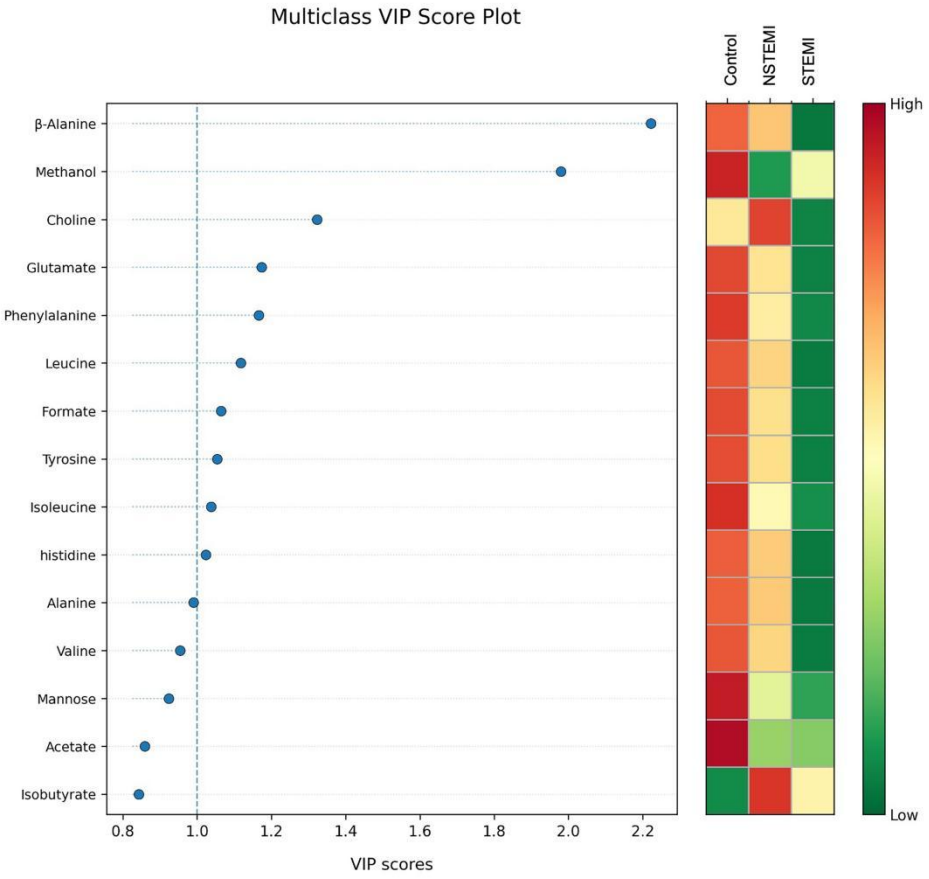


Figure S8. Multiclass VIP score plot of metabolites contributing to discrimination among the control, NSTEMI, and STEMI groups. Metabolites are ranked according to their VIP scores derived from the multiclass OPLS-DA model, with higher scores indicating a greater contribution to group discrimination. Each point represents the VIP score of an individual metabolite, and the vertical dashed line at VIP = 1.0 denotes the commonly applied threshold for identifying variables with an important contribution to the model. The adjacent heatmap displays the relative abundance of each metabolite across the three study groups, with warmer colors indicating higher relative abundance and cooler colors indicating lower relative abundance. VIP scores reflect model contribution and should not be interpreted independently as evidence of statistical significance. **Abbreviations:** NSTEMI, non-ST-segment elevation myocardial infarction; OPLS-DA, orthogonal projections to latent structures discriminant analysis; STEMI, ST-segment elevation myocardial infarction; VIP, variable importance in projection.