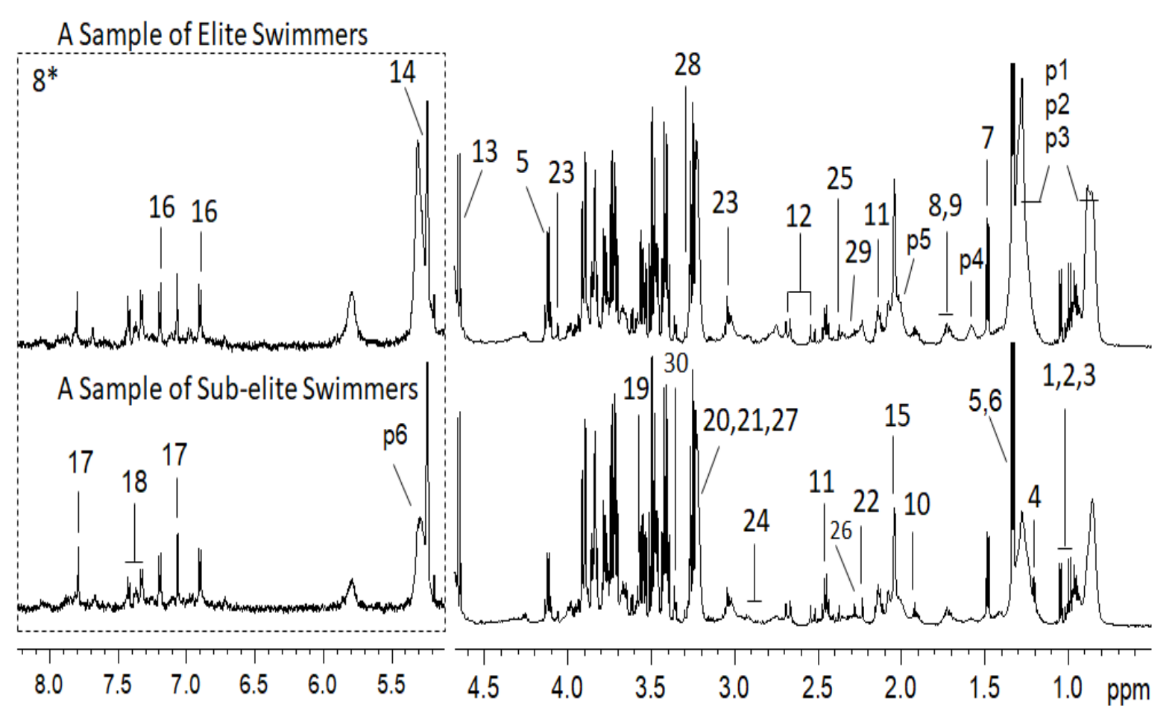
Supplementary Material

# Supplementary Figures and Tables

## Supplementary Figures



**Supplementary Figure 1.** Typical serum one-dimensional 1H NMR spectra.



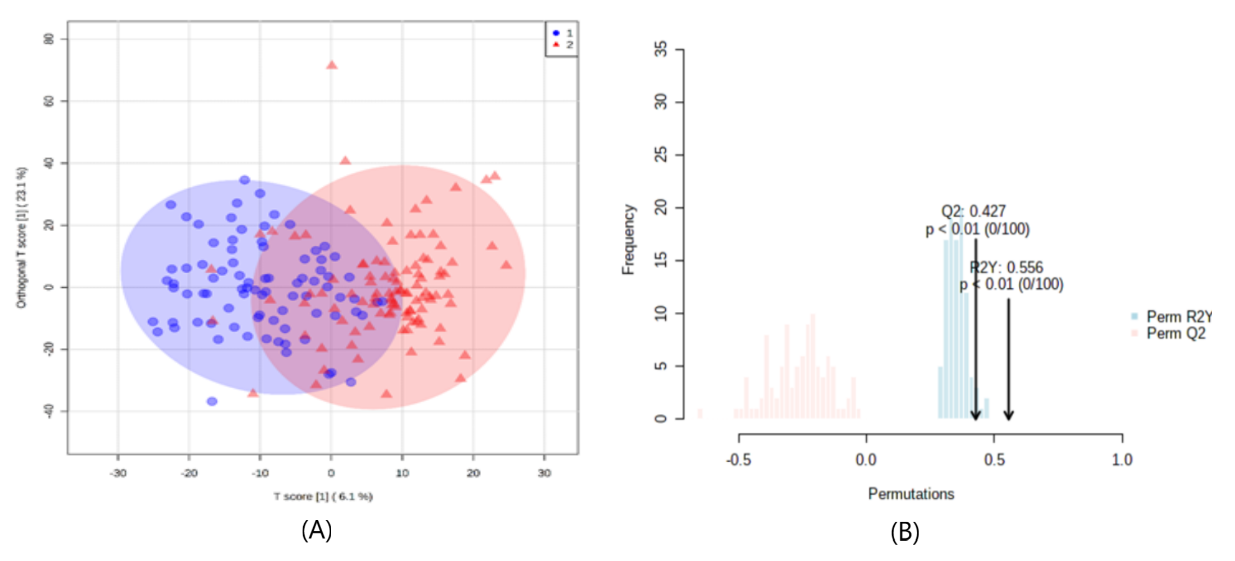
**Supplementary Figure 2.** Metabolites with distinct patterns between the two groups in male



**Supplementary Figure 3.** Metabolites with distinct patterns between the two groups in female



**Supplementary Figure 4.** LASSO regression analysis of serum metabolites



**Supplementary Figure 5.** OPLS-DA between sub-elite group and elite group using MetaboAnalyst.

## Supplementary Tables

**Supplementary Table 1** 1H NMR assignments for serum metabolites in swimmers

|  |  |  |  |
| --- | --- | --- | --- |
| No. | metabolites | moieties | δ 1H (ppm) and multiplicitya |
| 1 | Valine | αCH | 3.62(d) |
|  |  | βCH | 2.28(m) |
|  |  | γCH3 | 1.05(d) |
|  |  | γ′CH3 | 0.99 (d) |
|  |  | COOH |  |
| 2 | Isoleucine | αCH | 3.67(d) |
|  |  | βCH | 1.98(m) |
|  |  | γCH2 | 1.47(m) |
|  |  | γCH2' | 1.25(m) |
|  |  | γ′CH3 | 1.01(d) |
|  |  | δCH3 | 0.94 (t) |
|  |  | COOH |  |
| 3 | Leucine | αCH | 3.74(d) |
|  |  | βCH2 | 1.71(m) |
|  |  | γCH | 1.69(m) |
|  |  | δCH3 | 0.97(d) |
|  |  | δ′CH3 | 0.96(d) |
|  |  | COOH |  |
| 4 | 3-Hydroxybutytrate | αCH | 2.31(dd) |
|  |  | αCH' | 2.41(dd) |
|  |  | βCH2 | 4.16(m) |
|  |  | γCH3 | 1.20(d) |
| 5 | Lactate | αCH | 4.12(q) |
|  |  | βCH3 | 1.33(d) |
|  |  | COOH |  |
| 6 | Threonine | αCH | 3.59(d) |
|  |  | βCH2 | 4.26(m) |
|  |  | γCH3 | 1.33(d) |
|  |  | COOH |  |
| 7 | Alanine | αCH | 3.78(q) |
|  |  | βCH3 | 1.48(d) |
|  |  | COOH |  |
| 8 | Lysine | αCH | 3.76(t) |
|  |  | βCH2 | 1.90(m) |
|  |  | γCH2 | 1.46(m) |
|  |  | δCH2 | 1.71(m) |
|  |  | CH2 | 3.01(t) |
|  |  | COOH |  |
| 9 | Arginine | αCH | 3.78(t) |
|  |  | βCH2 | 1.92(m) |
|  |  | γCH2 | 1.68(m) |
|  |  | δCH2 | 3.24(t) |
|  |  | COOH |  |
| 10 | Acetate | CH3 | 1.92(s) |
|  |  | COOH |  |
| 11 | Glutamine | αCH | 3.77(t) |
|  |  | βCH2 | 2.14(m) |
|  |  | γCH2 | 2.46(m) |
|  |  | COOH |  |
|  |  | CO |  |
| 12 | Citrate | CH2 | 2.53(d) |
|  |  | CH2' | 2.68(d) |
|  |  | C-OH |  |
|  |  | COOH |  |
|  |  | COOH |  |
| 13 | β-Glucose | 1-CH | 4.65(d) |
|  |  | 2-CH | 3.26(dd) |
|  |  | 3-CH | 3.50(dd) |
|  |  | 4-CH | 3.40(dd) |
|  |  | 5-CH | 3.47(dd) |
|  |  | 6-CH | 3.74(dd) |
|  |  | 6′-CH | 3.90(dd) |
| 14 | α-Glucose | 1-CH | 5.24(d) |
|  |  | 2-CH | 3.54(dd) |
|  |  | 3-CH | 3.73(dd) |
|  |  | 4-CH | 3.42(dd) |
|  |  | 5-CH | 3.83(dd) |
|  |  | 6-CH2 | 3.83(dd) |
| 15 | N-Acetylated Glycoproteins (NAG) | CH3 | 2.04(s) |
| 16 | Tyrosine | 3 or 5-CH | 6.90(d) |
|  |  | 2 or 6-CH | 7.19(d) |
|  |  | αCH | 3.94(dd) |
|  |  | β′CH2 | 3.20(dd) |
|  |  | βCH2 | 3.07(dd) |
|  |  | C(ring) |  |
|  |  | C-OH(ring) |  |
|  |  | COOH |  |
| 17 | Histidine | 4-CH | 7.06(s) |
|  |  | 2-CH | 7.79(s) |
| 18 | Phenylalanine | 2 or 6-CH | 7.33(dd) |
|  |  | 3 or 5-CH | 7.43(dd) |
|  |  | 4-CH | 7.37(m) |
|  |  | βCH2 | 3.12(dd) |
|  |  | β′CH2 | 3.25(dd) |
|  |  | αCH | 3.98(dd) |
|  |  | COOH |  |
| 19 | Glycine | CH2 | 3.56(s) |
|  |  | COOH |  |
| 20 | Choline | N(CH3)3 | 3.20(s) |
|  |  | N-CH2 | 3.52(m) |
|  |  | O-CH2 | 4.07(m) |
| 21 | Phosphocholine | N(CH3)3 | 3.21(s) |
|  |  | N-CH2 | 3.59(m) |
|  |  | O-CH2 | 4.17(m) |
| 22 | Acetone | CH3 | 2.23(s) |
| 23 | Creatinine | CH3 | 3.05(s) |
|  |  | CH2 | 4.06(s) |
|  |  | C=NH |  |
|  |  | COOH |  |
| 24 | Asparagine | βCH2 | 2.86(dd) |
|  |  | βCH2' | 2.95(dd) |
|  |  | αCH | 4.00(dd) |
|  |  | COOH |  |
| 25 | Pyruvate | CH3 | 2.37(s) |
| 26 | Acetoacetate | CH3 | 2.28(s) |
|  |  | CH2 | 3.43(s) |
| 27 | Glycerophosphocholine | N(CH3)3 | 3.23(s) |
|  |  | N-CH2 | 3.66(m) |
|  |  | O-CH2 | 4.32(m) |
| 28 | Betaine | N(CH3)3 | 3.27(s) |
|  |  | OCH2 | 3.90(s) |
| 29 | Glutamate | αCH | 3.76(t) |
|  |  | βCH2 | 2.08(m) |
|  |  | γCH2 | 2.35(m) |
|  |  | COOH |  |
| 30 | Methanol | CH3 | 3.36(s) |
| 31 | HDL |  | 0.86(brs) |
| 32 | LDL |  | 0.88(brs) |
| 33 | VLDL |  | 0.90(brs) |
| 34 | Lipids |  | 1.59(brs) |
| 35 | Lipid (Unsatured Fatty Acids) |  | 2.00(brs) |
| 36 | Unsatured Fatty Acids |  | 5.30(brs) |

keys for multiplicity in parenthesis: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublet; brs, broad singlet.

**Supplementary Table 2** 36 serum metabolites between elite and sub-elite level swimmers in total, male and female

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Metabolites | Elite level swimmers vs.Sub-elite level swimmers | | | | | |
| Fold (Elite/Sub-elite,Total) | *P* value | Fold (Elite/Sub-elite,Male) | *P* value | Fold (Elite/Sub-elite,Female) | *P* value |
| Valine | 0.942 | 8.06E-02 | 0.937 | 1.30E-02 | 0.975 | 3.79E-01 |
| Isoleucine | 0.923 | 8.89E-04 | 0.894 | 2.24E-04 | 0.971 | 3.66E-01 |
| Leucine | 0.963 | 5.70E-02 | 0.947 | 2.32E-01 | 0.992 | 7.70E-01 |
| 3-hydroxybutyric acid | 0.904 | 3.22E-02 | 0.946 | 2.05E-01 | 0.826 | 2.40E-02 |
| Lactic acid | 1.123 | 3.39E-04 | 1.053 | 4.40E-02 | 1.195 | 4.89E-04 |
| Threonine | 0.975 | 4.48E-01 | 0.981 | 6.02E-01 | 0.969 | 2.07E-01 |
| Alanine | 1.010 | 7.05E-01 | 0.976 | 4.55E-01 | 1.076 | 1.18E-01 |
| Lysine | 1.015 | 4.18E-01 | 1.028 | 2.55E-01 | 1.016 | 5.25E-01 |
| Arginine | 0.967 | 1.14E-01 | 0.969 | 2.33E-01 | 0.996 | 8.87E-01 |
| Acetate | 0.964 | 1.28E-01 | 0.978 | 2.77E-01 | 0.968 | 1.82E-01 |
| Glutamine | 0.936 | 2.44E-05 | 0.929 | 1.15E-04 | 0.955 | 5.90E-02 |
| Citrate | 0.976 | 2.30E-01 | 0.955 | 1.75E-01 | 1.010 | 7.32E-01 |
| β-Glucose | 0.967 | 2.57E-01 | 0.961 | 2.18E-01 | 0.975 | 5.76E-01 |
| α-glucose | 0.931 | 4.09E-09 | 0.920 | 4.39E-07 | 0.945 | 4.46E-03 |
| N-Acetylated Glycoproteins | 0.943 | 1.98E-01 | 0.937 | 9.70E-02 | 0.947 | 2.16E-01 |
| Tyrosine | 0.969 | 1.11E-01 | 0.956 | 1.53E-01 | 1.008 | 8.09E-01 |
| Histidine | 0.993 | 6.04E-01 | 0.985 | 4.56E-01 | 1.017 | 4.04E-01 |
| Phenylalanine | 1.010 | 5.38E-01 | 1.006 | 7.85E-01 | 1.034 | 1.84E-01 |
| Glycine | 0.945 | 5.66E-04 | 0.934 | 2.04E-03 | 0.970 | 2.00E-01 |
| Choline | 1.001 | 9.53E-01 | 1.003 | 9.06E-01 | 1.030 | 2.79E-01 |
| Phosphocholine | 1.016 | 4.77E-01 | 1.013 | 6.49E-01 | 1.059 | 7.50E-02 |
| Acetone | 0.886 | 5.52E-02 | 0.924 | 4.02E-01 | 0.847 | 1.21E-01 |
| Creatinine | 1.011 | 5.17E-01 | 1.023 | 2.26E-01 | 1.039 | 1.66E-01 |
| Asparagine | 0.981 | 2.68E-01 | 0.991 | 6.84E-01 | 0.984 | 5.46E-01 |
| Pyruvate | 1.000 | 9.98E-01 | 0.976 | 4.78E-01 | 1.047 | 3.06E-01 |
| Acetoacetate | 0.934 | 2.78E-02 | 0.969 | 3.59E-01 | 0.887 | 7.00E-02 |
| Glycerophosphorylcholine | 1.063 | 8.28E-02 | 0.983 | 6.56E-01 | 1.081 | 1.54E-01 |
| Betaine | 1.016 | 3.66E-01 | 1.002 | 9.07E-01 | 1.071 | 1.17E-01 |
| Glutamate | 1.002 | 9.31E-01 | 0.991 | 6.83E-01 | 1.056 | 8.10E-02 |
| Methanol | 1.292 | 2.97E-04 | 1.213 | 2.50E-02 | 1.451 | 1.37E-03 |
| High-density lipoprotein | 1.123 | 8.63E-04 | 1.101 | 2.60E-02 | 1.148 | 8.00E-03 |
| Low-density lipoprotein | 0.961 | 4.00E-01 | 0.964 | 5.85E-01 | 0.960 | 5.68E-01 |
| Very low-density lipoprotein | 0.965 | 1.33E-01 | 0.954 | 2.21E-01 | 0.971 | 5.55E-01 |
| Lipids | 0.933 | 8.50E-02 | 0.920 | 4.23E-01 | 0.951 | 6.88E-01 |
| Lipid (Unsaturated Fatty Acids) | 0.958 | 2.57E-01 | 0.961 | 1.98E-01 | 0.951 | 2.34E-01 |
| Unsaturated fatty acids | 1.110 | 1.19E-02 | 1.059 | 3.03E-01 | 1.101 | 4.10E-02 |