Supplementary Material

**Supplementary Table 1** Summarize of metabolic differences in adolescents with different constitution states.

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| --- | --- | --- | --- | --- |
| **Ion mode** | **Metabolites** | **OB vs NW** | **OW vs NW** | **OB|OW vs NW** |
| POS | Differential metabolites (Up/ Down) | 477(324/153) | 330(239/91) | 398(190/208) |
| Known metabolites (Up/ Down) | 347(246/101) | 246(183/63) | 279(153/126) |
| NEG | Differential metabolites (Up/ Down) | 415(239/176) | 183(115/68) | 271(97/174) |
| Known metabolites (Up/ Down) | 123(60/63) | 27(13/14) | 68(15/53) |

POS, positive; NEG, negative; Up, upregulated; Down, downregulated; OB, obesity; OW, overweight； NW, normal-weight.

**Supplementary Table 2** Multiple linear regression analysis of SBP as dependent variable.

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| --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **β** | **SE** | **β(95%CI)** | **t** | ***P*** | ***F*** |
| Constants | 146.20 | 3.62 | **-** | 40.40 | 0.001 | F(3,101)=16.428,  *P*<0.001 |
| Sex | -12.74 | 2.29 | (-17.29,-8.20) | -5.56 | 0.001 |
| Triglyceride | 7.39 | 2.67 | ( 2.09,12.68 ) | 2.77 | 0.007 |
| OMS | 1.88 | 0.76 | ( 0.38,3.38 ) | 2.48 | 0.015 |

SBP, systolic blood pressure; OMS, Obesity-related metabolite score. Take SBP as the dependent variable, the stepwise multiple linear regression showed that after adjusting for age, sex, ethnicity, triglyceride, cholesterol, HDLC, LDLC, and OMS, the factors that independently influenced SBP were sex(*β* =-12.74, 95% CI:-17.29,-8.20, *P*=0.001), triglyceride (*β* = 7.39, 95% CI: 2.09,12.68, *P*=0.007), and OMS (*β* = 1.88, 95% CI: 0.38,3.38, *P*=0.015).

**Supplementary Table 3** Multiple linear regression analysis of DBP as dependent variable.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **β** | **SE** | **β(95%CI)** | **t** | ***P*** | ***F*** |
| Constants | 72.50 | 0.90 | **-** | 80.22 | 0.001 | F(1,103)=5.315,  *P*=0.023 |
| Triglyceride | 4.30 | 1.87 | (0.60,8.00) | 2.31 | 0.023 |

DBP, diastolic blood pressure; Take DBP as the dependent variable, the stepwise multiple linear regression showed that after adjusting for age, sex, ethnicity, triglyceride, cholesterol, HDLC, LDLC, and OMS, the factors that independently influenced DBP were triglyceride (*β* = 4.30, 95% CI: 0.60, 8.00, *P*=0.023).

图示

中度可信度描述已自动生成**Supplementary Figure 1** Restrictive cubic spline plot of 12 metabolites and BMI

图示, 示意图

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**Supplementary Figure 2** Boxplots of selected metabolites with significantly different concentrations between NW (red), OW (green), and AD (blue). ns: p > 0.05, \*: p <= 0.05, \*\*: p <= 0.01, \*\*\*: p <= 0.001.