

Supplementary Materials: Differential Amino Acid, Carbohydrate and Lipid Metabolism Perpetuations Involved in a Subtype of Rheumatoid Arthritis with Chinese Medicine Cold Pattern

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Table S1. Identified differential metabolites between rheumatoid arthritis (RA) cold pattern patients and healthy controls.

| Metabolite | ID | Fold Change (Cold vs. Control) | False Discovery Rate (FDR) <i>p</i> Value |
|---------------------------------|-----------|-----------------------------------|--|
| Up-Regulated | | | |
| Glycochenodeoxycholate | HMDB00637 | 3.33 | 0.009 |
| Phosphatidylethanolamine (38:6) | HMDB09454 | 1.43 | <0.001 |
| Phosphatidylethanolamine (32:1) | HMDB08827 | 1.43 | <0.001 |
| Lysophosphatidylcholine (18:2) | HMDB10386 | 1.43 | <0.001 |
| L-valine | HMDB00883 | 1.25 | 0.008 |
| Phosphatidylcholine (34:2) | HMDB07880 | 1.25 | 0.026 |
| Phosphatidylcholine (36:4) | HMDB07889 | 1.25 | 0.003 |
| Phosphatidylcholine (36:5) | HMDB07891 | 1.25 | 0.007 |
| Phosphatidylcholine (34:3) | HMDB07881 | 1.25 | 0.007 |
| L-threonine | HMDB00167 | 1.11 | 0.041 |
| L-isoleucine | HMDB00172 | 1.11 | 0.011 |
| Down-Regulated | | | |
| Palmitic acid | HMDB00220 | 0.83 | 0.001 |
| Cholesterol | HMDB00067 | 0.83 | <0.001 |
| Linoleic acid | HMDB00673 | 0.83 | 0.011 |
| D-alanine | HMDB01310 | 0.83 | 0.014 |
| Urea | HMDB00294 | 0.77 | 0.001 |
| Stearic acid | HMDB00827 | 0.77 | <0.001 |
| Citric acid | HMDB00094 | 0.77 | 0.013 |
| Phosphatidylcholine (32:1) | HMDB13404 | 0.77 | 0.026 |
| Tetradecanoylcarnitine | HMDB05066 | 0.77 | 0.006 |
| Hexadecanoylcarnitine | HMDB06210 | 0.77 | 0.002 |
| D-glucose | HMDB00122 | 0.71 | <0.001 |
| Myoinositol | HMDB00211 | 0.67 | <0.001 |
| Dodecanoylcarnitine | HMDB00651 | 0.67 | 0.016 |
| Oleic acid | HMDB00207 | 0.59 | <0.001 |
| Carnitine | HMDB00062 | 0.59 | 0.018 |
| 3-hydroxybutyric acid | HMDB00357 | 0.50 | 0.013 |
| L-proline | HMDB00162 | 0.40 | <0.001 |
| D-glyceric acid | HMDB00139 | 0.29 | <0.001 |

Table S2. Identified differential metabolites between RA heat pattern patients and healthy controls

| Metabolite | ID | Fold Change (Heat vs. Control) | False Discovery Rate (FDR) <i>p</i> Value |
|---------------------------------|-----------|-----------------------------------|--|
| Up-Regulated | | | |
| Lysophosphatidylcholine (18:2) | HMDB10386 | 1.43 | <0.001 |
| Phosphatidylethanolamine (38:6) | HMDB09454 | 1.43 | <0.001 |
| L-valine | HMDB00883 | 1.25 | 0.002 |
| L-threonine | HMDB00167 | 1.25 | 0.036 |
| L-leucine | HMDB00687 | 1.25 | 0.043 |
| Phosphatidylcholine (34:2) | HMDB07880 | 1.25 | 0.042 |
| Phosphatidylcholine (34:3) | HMDB07881 | 1.25 | 0.029 |
| L-isoleucine | HMDB00172 | 1.11 | 0.038 |
| Down-Regulated | | | |
| Phosphatidylcholine (32:0) | HMDB07871 | 0.83 | 0.002 |
| Oleic acid | HMDB00207 | 0.71 | 0.009 |
| D-alanine | HMDB01310 | 0.71 | 0.01 |
| Phosphatidylcholine(34:1) | HMDB07879 | 0.71 | <0.001 |
| Myoinositol | HMDB00211 | 0.67 | <0.001 |
| D-glucose | HMDB06564 | 0.67 | <0.001 |
| Carnitine | HMDB00062 | 0.63 | 0.008 |
| Phosphatidylcholine (32:1) | HMDB13404 | 0.56 | <0.001 |
| L-proline | HMDB03411 | 0.45 | <0.001 |
| D-glyceric acid | HMDB00139 | 0.34 | 0.001 |
| Phytosphingosine | HMDB04610 | 0.31 | 0.029 |

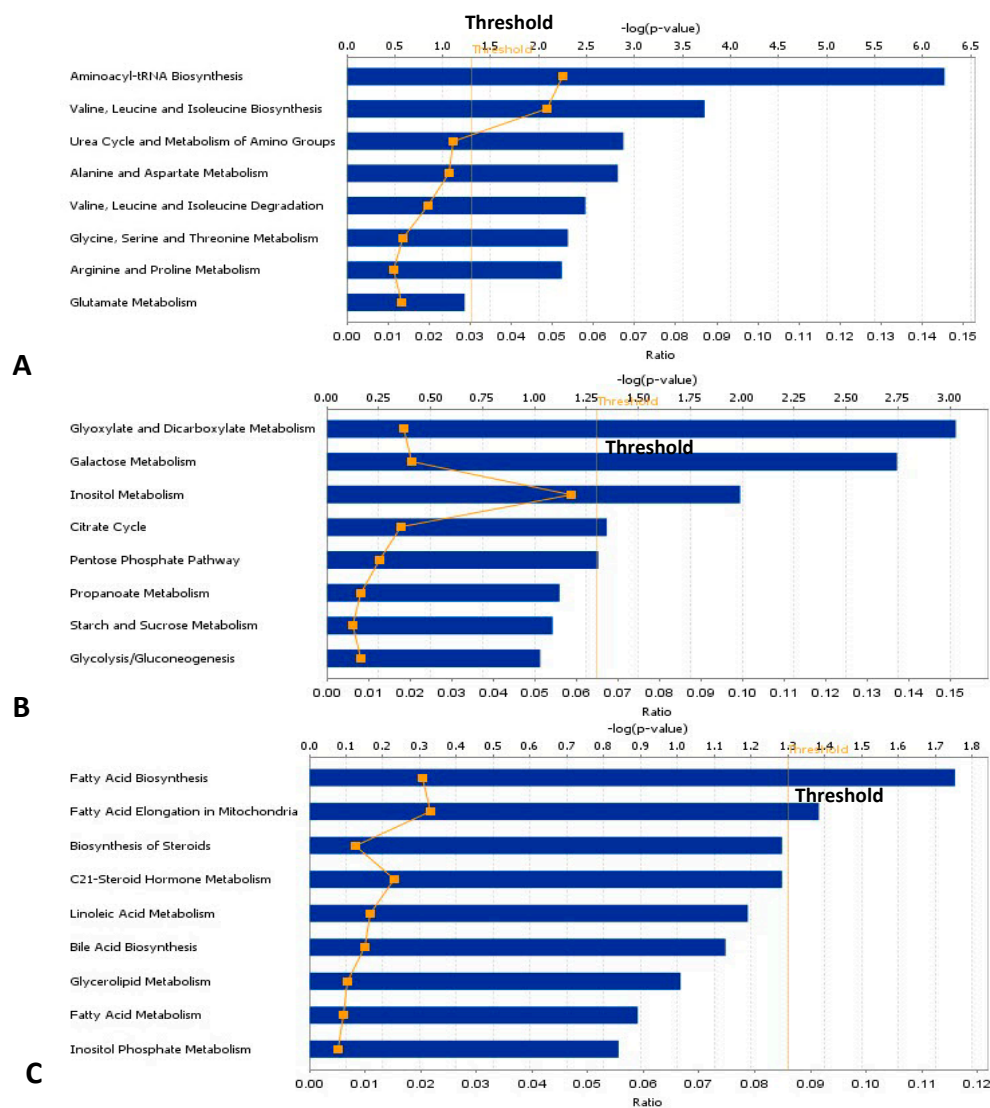


Figure S1. The canonical pathways involved in amino acids, carbohydrates and lipids metabolism between RA cold pattern patients and healthy controls. (A) amino acids metabolism related pathway; (B) carbohydrates metabolism related pathway; (C) lipids metabolism related pathway.

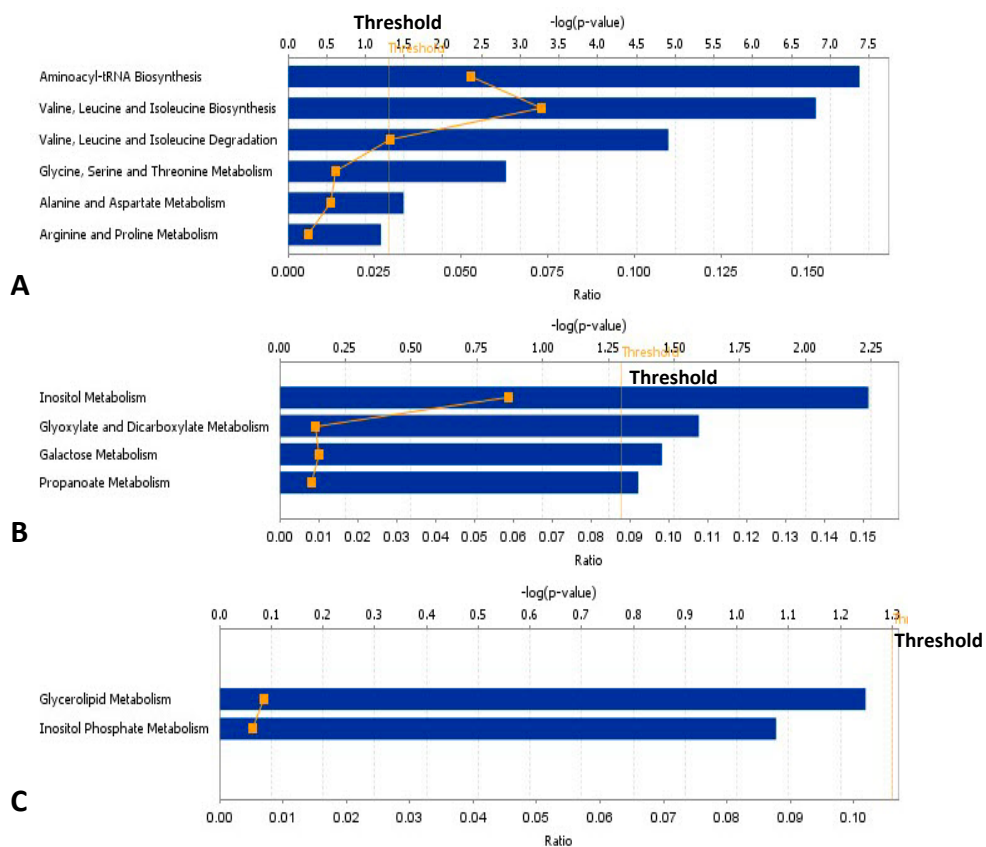


Figure S2. The canonical pathways involved in amino acids, carbohydrates and lipids between RA heat pattern patients and healthy controls. (A) amino acids metabolism related pathway; (B) carbohydrates metabolism related pathway; (C) lipids metabolism related pathway.