**Supplementary Material**

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## Supplementary table 1. Classification criteria of DBI-16 indicators

|  |  |
| --- | --- |
| DBI-16 indicators | DBI component scores |
|  |
| HBS |  |  |
| almost no diet problem | 0-9 |  |
| low level | 10-18 |  |
| moderate level | 19-27 |  |
| high level | >27 |  |
| LBS |  |  |
| almost no diet problem | 0-14 |  |
| low level | 15-28 |  |
| moderate level | 29-43 |  |
| high level | >43 |  |
| DQD |  |  |
| almost no diet problem | 0-19 |  |
| low level | 20-38 |  |
| moderate level | 39-57 |  |
| high level | >57 |  |

Abbreviations: HBS, high bound score; LBS, low bound score; DQD, diet quality distance.

## Supplementary table 2. The variance inflation factor (VIF) of multiple linear regression in this study

|  |  |  |
| --- | --- | --- |
| Independent variable | Adjustment | VIF |
| Metabolic profiles in pregnancy selected by LASSO | | |
|  | No | 1.31 |
| Yes | 1.34 |
| “Meat-Cereal-Vegetable” pattern | | |
|  | No | 1.51 |
| Yes | 1.23 |
| “Nut-Soybean” pattern | | |
|  | No | 1.51 |
| Yes | 1.24 |
| DBI-HBS | | |
|  | No | 1.01 |
| Yes | 1.11 |
| DBI-LBS | | |
|  | No | 1.85 |
| Yes | 1.44 |
| DBI-DQD | | |
|  | No | 1.97 |
| Yes | 1.41 |
| Metabolic profiles in pregnancy and dietary patterns during lactation selected by LASSO | | |
|  | No | 1.45 |
| Yes | 1.39 |

Abbreviations: VIF, variance inflation factor; LASSO, least absolute shrinkage and selection operator; HBS, high bound score; LBS, low bound score; DQD, diet quality distance.

## Supplementary table 3. Metabolic characteristics in pregnancy of participants

|  |  |
| --- | --- |
| Characteristics | Value (n=295) \* |
| Protein metabolism |  |
| TP (g/L) | 66.1 (64.3-68.5) |
| ALB (g/L) | 36.4 (35.1-37.9) |
| GLB (g/L) | 30.0 (28.3-31.6) |
| Glucolipid metabolism |  |
| GLU (mmol/L) | 4.25 (4.02-4.52) |
| TG (mmol/L) | 2.11 (1.74-2.64) |
| TC (mmol/L) | 6.19 (5.53-6.76) |
| HDL-C (mmol/L) | 2.01 (1.79-2.21) |
| LDL-C (mmol/L) | 3.48 (3.01-3.93) |
| Calcium and phosphorous metabolism |  |
| Ca (mmol/L) | 2.24 (2.20-2.30) |
| IP (mmol/L) | 1.20 (1.13-1.27) |
| Bilirubin metabolism |  |
| TBIL (umol/L) | 9.0 (7.7-10.9) |
| DBIL (umol/L) | 2.8 (2.3-3.4) |
| IBIL (umol/L) | 6.3 (5.5-7.6) |
| Enzymatic activity |  |
| ALT (U/L) | 15 (12-22) |
| AST (U/L) | 18 (15-22) |
| GGT (U/L) | 11 (9-14) |
| ALP (U/L) | 63 (54-72) |
| LDH (U/L) | 154 (140-172) |
| α-HBDH (U/L) | 126 (106-143) |
| CK (U/L) | 39 (31-49) |
| Renal function |  |
| Urea (mmol/L) | 2.88 (2.42-3.29) |
| CRE (umol/L) | 46 (42-50) |
| UA (umol/L) | 243 (212-274) |

Abbreviations: TP, total protein; ALB, albumin; GLB, globulin; GLU, glucose; TG, triglyceride; TC, total cholesterol; HDL-C, high-density lipoprotein cholesterol; LDL-C, low-density lipoprotein cholesterol; IP, inorganic phosphorus; TBIL, total bilirubin; DBIL, direct bilirubin; IBIL, indirect bilirubin; ALT, alanine aminotransferase; AST, aspartate aminotransferase; GGT, gamma-glutamyl transferase; ALP, alkaline phosphatase; LDH, lactate dehydrogenase; α-HBDH, alpha-hydroxybutyrate dehydrogenase; CK, creatine kinase; CRE, creatinine; UA, uric acid.

\* Values were median (IQR).

## Supplementary table 4. Participants’ dietary intakes during lactation

|  |  |
| --- | --- |
| Food groups | Intakes (n = 270)\* |
| Cereal (g/d) | 205 (146-300) |
| Tuber (g/d) | 21 (5-50) |
| Soybean (g/d) | 29 (10-72) |
| Vegetable (g/d) | 471 (296-675) |
| Fungi and algae (g/d) | 10 (0-43) |
| Fruit (g/d) | 201 (100-300) |
| Nut and seed (g/d) | 3 (0-13) |
| Meat and poultry (g/d) | 95 (55-171) |
| Milk (g/d) | 200 (54-250) |
| Egg (g/d) | 79 (60-120) |
| Fish and shrimp (g/d) | 21 (8-43) |
| Snack (g/d) | 0 (0-3) |
| Beverage (g/d) | 0 (0-4) |
| Oil (g/d) | 20 (18-25) |
| Condiment (g/d) | 11 (0-21) |

\* Values were median (IQR).

## Supplementary table 5 Dietary intake of “Meat-Vegetable-Cereal” pattern during lactation

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Food groups/  Nutritional component | “Meat-Vegetable-Cereal” pattern\* | | | | rs | *P* value |
| Q1 (n = 67) | Q2 (n = 68) | Q3 (n = 68) | Q4 (n = 67) |
| Food groups |  |  |  |  |  |  |
| Cereal(g/d) | 150 (95-200) | 199 (151-286) | 230 (164-308) | 300 (210-425) | 0.45 | <0.001 |
| Tuber(g/d) | 14 (3-29) | 29 (4-65) | 21 (7-46) | 23 (5-58) | 0.04 | 0.468 |
| Soybean(g/d) | 18 (6-79) | 27 (9-57) | 32 (15-73) | 44 (14-86) | 0.17 | 0.005 |
| Vegetable(g/d) | 280 (143-337) | 405 (269-587) | 599 (457-804) | 671 (486-975) | 0.58 | <0.001 |
| Fungi and algae(g/d) | 3 (0-29) | 9 (0-32) | 16 (0-43) | 29 (0-200) | 0.20 | 0.001 |
| Fruit(g/d) | 200 (88-300) | 204 (113-300) | 213 (143-308) | 200 (86-300) | 0.00 | 0.944 |
| Nut and seed(g/d) | 2 (0-15) | 5 (0-15) | 3 (0-11) | 6 (0-13) | -0.01 | 0.902 |
| Meat and poultry(g/d) | 48 (31-66) | 86 (66-113) | 144 (90-187) | 195 (107-273) | 0.65 | <0.001 |
| Milk(g/d) | 250 (71-400) | 165 (56-250) | 200 (49-250) | 125 (6-250) | -0.14 | 0.025 |
| Egg(g/d) | 88 (60-150) | 100 (60-130) | 70 (60-120) | 65 (50-120) | -0.15 | 0.016 |
| Fish and shrimp(g/d) | 8 (2-18) | 15 (9-35) | 29 (14-43) | 62 (21-126) | 0.56 | <0.001 |
| Snack(g/d) | 0 (0-4) | 0 (0-1) | 0 (0-4) | 0 (0-4) | 0.02 | 0.712 |
| Beverage(g/d) | 0 (0-14) | 0 (0-4) | 0 (0-3) | 0 (0-0) | -0.13 | 0.028 |
| Oil(g/d) | 20 (18-25) | 20 (18-25) | 20 (17-25) | 25 (18-45) | 0.16 | 0.007 |
| Condiment(g/d) | 5 (0-15) | 11 (0-21) | 15 (6-21) | 13 (0-26) | 0.22 | <0.001 |
| Nutritional component† |  |  |  |  |  |  |
| Energy(kcal/d) | 1377 (1038-1915) | 1549 (1342-1835) | 1810 (1594-2162) | 2248 (2029-2781) | 0.54 | <0.001 |
| Protein(g/d) | 86.0 (77.8-94.5) | 89.5 (80.8-96.6) | 95.0 (83.5-104.4) | 92.5 (79.4-114.3) | 0.19 | 0.002 |
| Fat(g/d) | 85.3 (72.7-97.9) | 81.6 (65.9-93.1) | 75.8 (61.1-90.6) | 68.9 (50.8-97.3) | -0.20 | 0.001 |
| CHO(g/d) | 199.8 (174.3-232.6) | 214.2 (186.9-241.9) | 216.6 (178.1-242.5) | 219.9 (162.7-253.6) | 0.10 | 0.116 |
| Dietary fiber(g/d) | 13.0 (9.7-15.2) | 14.7 (11.3-17.6) | 16.5 (13.2-19.0) | 15.1 (11.4-23.2) | 0.21 | 0.001 |
| Cholesterol(mg/d) | 229 (151-283) | 248 (174-330) | 331 (210-427) | 335 (172-520) | 0.25 | <0.001 |
| Vitamin A(μgRAE/d) | 2184 (1534-3696) | 2121 (1379-5792) | 2614 (1175-6837) | 2338 (950-6883) | 0.10 | 0.096 |
| Thiamin(mg/d) | 0.98 (0.88-1.07) | 1.04 (0.92-1.15) | 1.09 (1.00-1.22) | 1.08 (0.89-1.26) | 0.26 | <0.001 |
| Riboflavin(mg/d) | 2.07 (1.71-2.70) | 2.06 (1.68-3.11) | 2.30 (1.62-3.29) | 1.86 (1.46-3.15) | -0.01 | 0.911 |
| Niacin(mg/d) | 14.80 (10.98-17.25) | 17.68 (14.91-20.42) | 20.30 (16.96-24.94) | 21.50 (16.70-30.62) | 0.49 | <0.001 |
| Vitamin C(mg/d) | 134.05 (82.90-171.69) | 179.38 (116.84-236.35) | 231.94 (178.67-270.53) | 227.57 (158.09-342.39) | 0.41 | <0.001 |
| Vitamin E(mg/d) | 23.58 (19.98-29.93) | 27.39 (22.73-33.63) | 27.18 (20.43-32.54) | 28.97 (25.01-35.69) | 0.20 | 0.001 |
| Ca(mg/d) | 845 (696-1008) | 787 (683-941) | 869 (681-1016) | 871 (608-1079) | 0.00 | 0.950 |
| P(mg/d) | 1419 (1296-1603) | 1438 (1359-1624) | 1536 (1384-1702) | 1519 (1291-1831) | 0.15 | 0.011 |
| K(mg/d) | 3015 (2432-3493) | 3226 (2691-3652) | 3446 (3017-4010) | 3521 (2622-4574) | 0.24 | <0.001 |
| Na(mg/d) | 2459.8 (1369.2-3690.8) | 3449.7 (1382.2-3922.3) | 3450.8 (2706.0-4007.5) | 3348.8 (1161.4-4694.9) | 0.10 | 0.107 |
| Mg(mg/d) | 380 (330-457) | 459 (386-505) | 538 (426-605) | 559 (433-684) | 0.44 | <0.001 |
| Fe(mg/d) | 25.5 (21.6-30.6) | 29.9 (23.2-39.7) | 34.3 (26.7-45.9) | 38.0 (25.2-52.0) | 0.32 | <0.001 |
| Zn(mg/d) | 10.31 (8.86-11.73) | 11.96 (10.47-13.03) | 13.88 (12.21-14.96) | 14.85 (11.52-17.41) | 0.53 | <0.001 |
| Se(μg/d) | 44.68 (37.85-54.85) | 56.69 (46.53-68.3) | 66.32 (53.72-79.85) | 74.02 (54.88-87.68) | 0.48 | <0.001 |
| Cu(mg/d) | 1.55 (1.36-1.83) | 1.64 (1.40-1.98) | 1.68 (1.50-1.90) | 1.71 (1.34-2.17) | 0.13 | 0.038 |
| Mn(mg/d) | 3.62 (2.78-4.20) | 4.49 (3.45-5.46) | 4.79 (4.00-5.52) | 5.19 (4.02-6.46) | 0.39 | <0.001 |

\* Values represent median (IQR).

† Nutrient intakes adjusted by energy using the residual method.

## Supplementary table 6. Dietary intake of “Nut-Soybean” pattern during lactation

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Food groups/  Nutritional component | “Nut-Soybean” pattern\* | | | | rs | *P* value |
| Q1 (n = 67) | Q2 (n = 68) | Q3 (n = 68) | Q4 (n = 67) |
| Food groups |  |  |  |  |  |  |
| Cereal (g/d) | 198 (129-275) | 211 (145-300) | 222 (152-312) | 218 (150-376) | 0.13 | 0.030 |
| Tuber (g/d) | 4 (0-20) | 21 (7-40) | 29 (12-59) | 35 (11-89) | 0.38 | <0.001 |
| Soybean (g/d) | 7 (0-19) | 30 (16-64) | 42 (20-98) | 55 (21-114) | 0.44 | <0.001 |
| Vegetable (g/d) | 457 (300-680) | 497 (300-664) | 500 (264-686) | 428 (300-600) | -0.05 | 0.369 |
| Fungi and algae (g/d) | 0 (0-36) | 11 (0-72) | 14 (0-42) | 14 (0-43) | 0.12 | 0.041 |
| Fruit (g/d) | 191 (71-250) | 200 (113-250) | 200 (99-331) | 250 (175-407) | 0.28 | <0.001 |
| Nut and seed (g/d) | 0 (0-0) | 3 (0-10) | 7 (2-15) | 15 (6-32) | 0.58 | <0.001 |
| Meat and poultry (g/d) | 75 (38-163) | 87 (60-161) | 113 (53-182) | 100 (57-176) | 0.12 | 0.044 |
| Milk (g/d) | 71 (0-200) | 250 (93-280) | 200 (57-250) | 250 (86-450) | 0.29 | <0.001 |
| Egg (g/d) | 60 (43-120) | 90 (60-125) | 70 (60-120) | 100 (60-143) | 0.13 | 0.037 |
| Fish and shrimp (g/d) | 14 (6-36) | 21 (8-40) | 23 (9-43) | 38 (14-64) | 0.23 | <0.001 |
| Snack (g/d) | 0 (0-0) | 0 (0-1) | 0 (0-7) | 1 (0-17) | 0.35 | <0.001 |
| Beverage (g/d) | 0 (0-0) | 0 (0-0) | 0 (0-22) | 0 (0-33) | 0.23 | <0.001 |
| Oil (g/d) | 20 (16-25) | 20 (17-25) | 20 (20-30) | 25 (20-45) | 0.28 | <0.001 |
| Condiment (g/d) | 0 (0-6) | 6 (0-16) | 15 (0-21) | 22 (12-32) | 0.52 | <0.001 |
| Nutritional component† |  |  |  |  |  |  |
| Energy (kcal/d) | 1448 (976-1794) | 1730 (1329-2050) | 1835 (1501-2282) | 2157 (1828-2682) | 0.50 | <0.001 |
| Protein (g/d) | 94.1 (84.1-101.8) | 93.8 (86.1-104.1) | 90.6 (77.7-102.2) | 84.4 (74.4-95.4) | -0.24 | <0.001 |
| Fat (g/d) | 71.2 (60.1-85.2) | 75.4 (61.5-89.2) | 82.7 (68.5-95.3) | 89.4 (68-103.7) | 0.25 | <0.001 |
| CHO (g/d) | 224.9 (191-249.4) | 214.6 (180.3-244.4) | 197.9 (167.9-244.2) | 197.2 (151.4-240.7) | -0.18 | 0.003 |
| Dietary fiber (g/d) | 14.8 (11.6-17.5) | 14.8 (12.3-17.3) | 15.2 (11.3-18.4) | 13.9 (10.3-19.6) | -0.04 | 0.494 |
| Cholesterol (mg/d) | 289 (205-387) | 284 (195-353) | 282 (187-563) | 195 (128-335) | -0.17 | 0.006 |
| Vitamin A (μgRAE/d) | 3833 (1953-7634) | 3569 (1498-6108) | 2072 (1078-3539) | 1400 (709-2798) | -0.34 | <0.001 |
| Thiamin (mg/d) | 1.08 (0.98-1.22) | 1.08 (1.00-1.16) | 1.07 (0.94-1.22) | 0.91 (0.76-1.00) | -0.31 | <0.001 |
| Riboflavin (mg/d) | 2.53 (1.75-3.36) | 2.46 (1.82-3.13) | 1.97 (1.39-2.69) | 1.78 (1.38-2.55) | -0.25 | <0.001 |
| Niacin (mg/d) | 18.76 (15.74-24.74) | 18.09 (15.00-22.63) | 17.85 (14.01-21.88) | 16.12 (10.92-21.06) | -0.18 | 0.004 |
| Vitamin C (mg/d) | 188.14 (137.70-270.38) | 198.70 (140.01-251.82) | 183.70 (109.73-242.76) | 176.41 (110.50-227.57) | -0.14 | 0.024 |
| Vitamin E (mg/d) | 23.29 (20.15-28.02) | 25.08 (21.16-29.43) | 28.91 (24.03-34.56) | 29.40 (23.31-38.90) | 0.27 | <0.001 |
| Ca (mg/d) | 783 (655-944) | 872 (713-1033) | 819 (630-1013) | 859 (672-1019) | 0.04 | 0.490 |
| P (mg/d) | 1473 (1298-1583) | 1519 (1379-1672) | 1492 (1254-1714) | 1481 (1302-1655) | 0.00 | 0.968 |
| K (mg/d) | 3222 (2754-3749) | 3341 (2955-3872) | 3320 (2602-3982) | 3233 (2506-3871) | -0.02 | 0.764 |
| Na (mg/d) | 1525.1 (1104.5-3400.1) | 3423.1 (1454.4-3922.0) | 3384.1 (1533.0-4053.3) | 3512.7 (2946.3-4485.5) | 0.29 | <0.001 |
| Mg (mg/d) | 488 (397-591) | 466 (402-597) | 479 (370-557) | 435 (362-536) | -0.13 | 0.032 |
| Fe (mg/d) | 35.8 (25.8-45.4) | 31.5 (24.5-42.5) | 29.0 (23.0-37.4) | 26.6 (19.9-35.0) | -0.25 | <0.001 |
| Zn (mg/d) | 12.69 (10.56-14.85) | 12.18 (10.80-14.79) | 12.98 (11.26-14.92) | 11.40 (9.22-12.70) | -0.17 | 0.005 |
| Se (μg/d) | 55.24 (43.97-73.11) | 59.04 (48.61-72.29) | 62.68 (46.09-76.60) | 59.75 (42.32-77.24) | 0.04 | 0.551 |
| Cu (mg/d) | 1.58 (1.42-1.80) | 1.63 (1.40-1.74) | 1.78 (1.45-2.09) | 1.71 (1.24-2.34) | 0.15 | 0.016 |
| Mn (mg/d) | 4.37 (3.61-5.46) | 4.59 (3.66-5.35) | 4.35 (3.37-5.68) | 4.50 (2.68-5.40) | -0.06 | 0.333 |

\* Values represent median (IQR).

† Nutrient intakes adjusted by energy using the residual method.

## Supplementary table 7. Characteristics of DBI-16 indicators in this study

|  |  |  |  |
| --- | --- | --- | --- |
| DBI-16 indicators | n (%) | Leptin (pg/ml) | |
| Median (IQR) | *P* value\* |
| HBS |  |  | 0.313 |
| almost no diet problem | 218 (80.7%) | 275.13 (126.56-537.91) |  |
| low level | 41 (15.2%) | 217.64 (69.10-402.60) |  |
| moderate/high level | 11 (4.1%) | 463.15 (120.41-745.94) |  |
| LBS |  |  | 0.289 |
| almost no diet problem | 51 (18.9%) | 320.17 (162.33-737.55) |  |
| low level | 126 (46.7%) | 266.56 (96.06-525.03) |  |
| moderate/high level | 93 (34.4%) | 237.31 (125.61-486.78) |  |
| DQD |  |  | 0.012 |
| almost no diet problem | 41 (15.2%) | 417.88 (187.67-731.57) |  |
| low level | 163 (60.4%) | 253.48 (96.06-485.78) |  |
| moderate/high level | 66 (24.4%) | 241.67 (121.29-601.92) |  |

Abbreviations: HBS, high bound score; LBS, low bound score; DQD, diet quality distance.

\* Kruskal-Wallis tests were used for group comparisons.

**Supplementary figure 1.** DAG for the association of human milk leptin with maternal metabolism in pregnancy and diet during lactation



Abbreviations: DAG, directed acyclic graph.

**Supplementary figure 2.** Spearman correlation analyses among 23 metabolic profiles



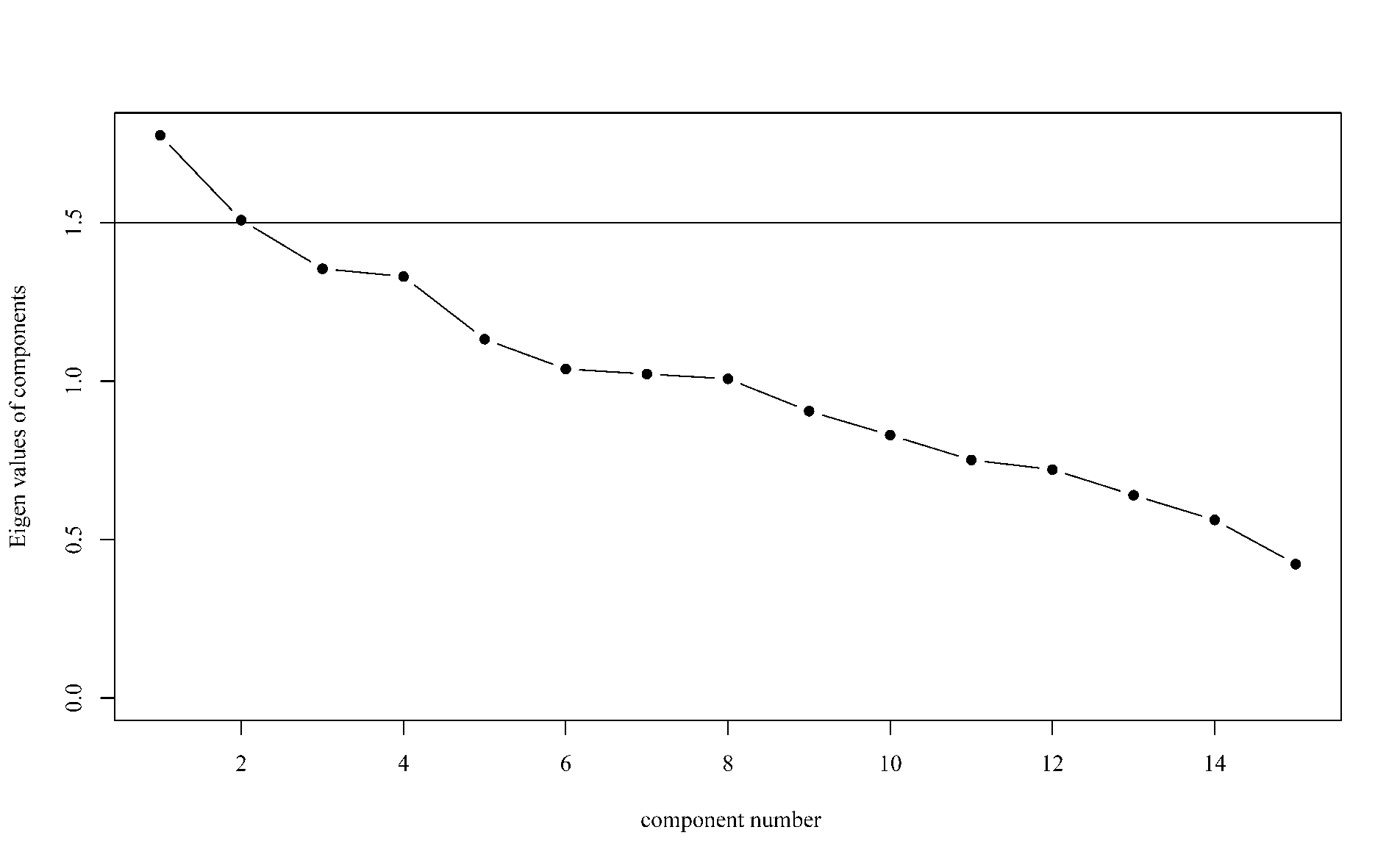
Abbreviations: TP, total protein; ALB, albumin; GLB, globulin; GLU, glucose; TG, triglyceride; TC, total cholesterol; HDL-C, high-density lipoprotein cholesterol; LDL-C, low-density lipoprotein cholesterol; IP, inorganic phosphorus; TBIL, total bilirubin; DBIL, direct bilirubin; IBIL, indirect bilirubin; ALT, alanine aminotransferase; AST, aspartate aminotransferase; GGT, gamma-glutamyl transferase; ALP, alkaline phosphatase; LDH, lactate dehydrogenase; α-HBDH, alpha-hydroxybutyrate dehydrogenase; CK, creatine kinase; CRE, creatinine; UA, uric acid.

**Supplementary figure 3.** Importance of selected variables of 23 metabolic profiles in pregnancy associated with breast milk leptin using LASSO regression model

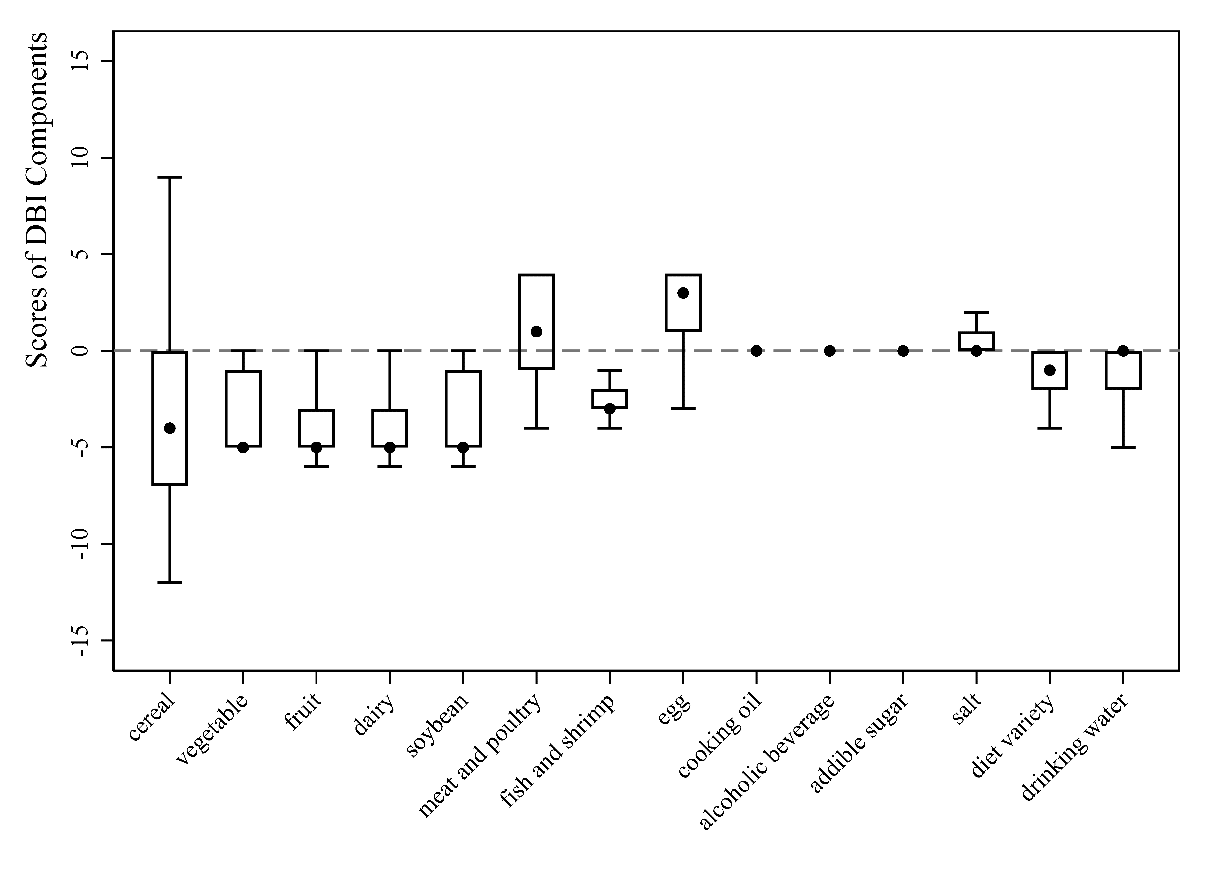


Abbreviations: GLU, glucose; ALB, albumin; GGT, gamma-glutamyl transferase; LDH, lactate dehydrogenase; TP, total protein; CK, creatine kinase; AST, aspartate aminotransferase; LDL-C, low-density lipoprotein cholesterol; ALT, alanine aminotransferase; CRE, creatinine; ALP, alkaline phosphatase; HDL-C, high-density lipoprotein cholesterol; UA, uric acid; TBIL, total bilirubin; α-HBDH, alpha-hydroxybutyrate dehydrogenase; IBIL, indirect bilirubin; GLB, globulin; IP, inorganic phosphorus; TG, triglyceride; DBIL, direct bilirubin; TC, total cholesterol.

**Supplementary figure 4.** Scree plot of PCA



**Supplementary figure 5.** Characteristics of DBI-16 components scores



**Supplementary figure 6.** Importance of selected variables of 28 predictors associated with breast milk leptin using LASSO regression model considering joint effect of metabolism in pregnancy and dietary patterns during lactation



Abbreviations: GLU, glucose; ALB, albumin; GGT, gamma-glutamyl transferase; TP, total protein; DQD, diet quality distance; LDH, lactate dehydrogenase; CK, creatine kinase; LDL-C, low-density lipoprotein cholesterol; UA, uric acid; LBS, low bound score; IBIL, indirect bilirubin; DBIL, direct bilirubin; HBS, high bound score; ALT, alanine aminotransferase; HDL-C, high-density lipoprotein cholesterol; TBIL, total bilirubin; CRE, creatinine; AST, aspartate aminotransferase; GLB, globulin; TG, triglyceride; α-HBDH, alpha-hydroxybutyrate dehydrogenase; IP, inorganic phosphorus; ALP, alkaline phosphatase; TC, total cholesterol.