*Article*

# Metabolic Signatures of Gestational Weight Gain and Postpartum Weight Loss in a Lifestyle Intervention Study of Overweight and Obese Women

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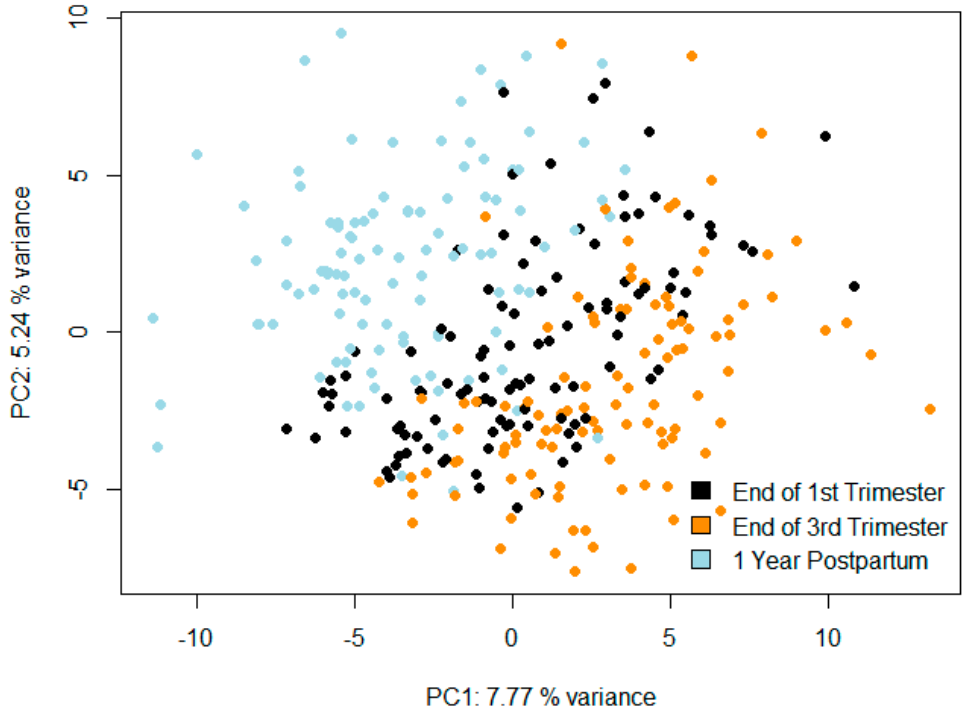
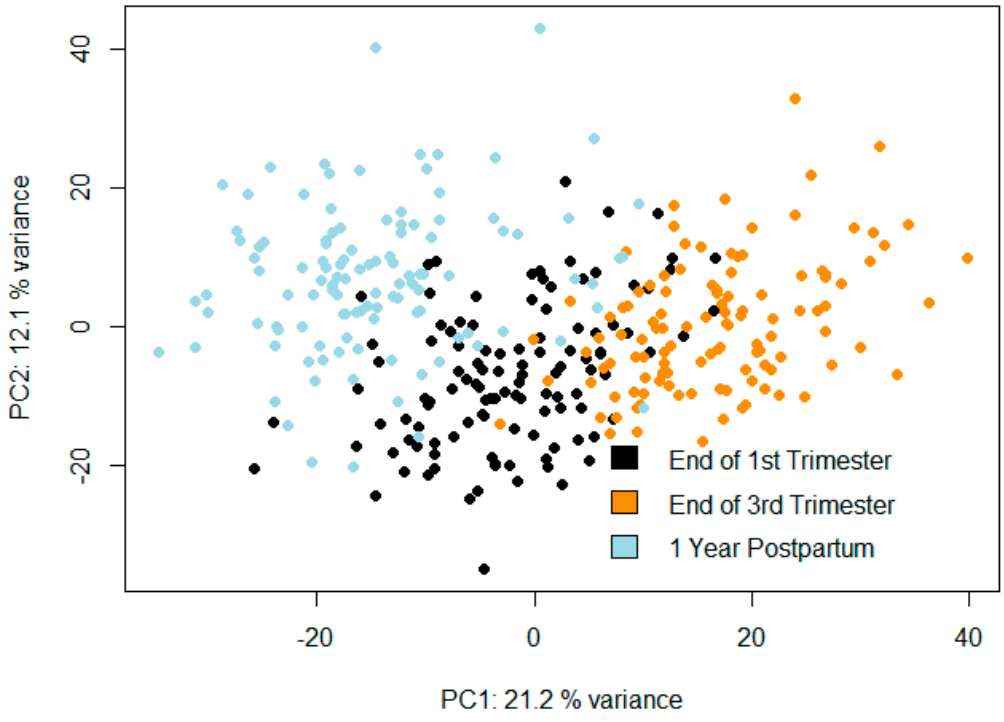



**Supplementary Figure S1 Principal Component Analysis of NMR urine samples.**




**Supplementary Figure S2 Principal Component Analysis of LC-MS plasma samples.**

**Supplementary Table S1 Details of Lipid annotations.**

| Lipid | RT(min) | m/z | Annotation | Confidence of Annotation |
|---|---|---|---|---|
| LPS(O-18:0) | 1.64 | 512.34 | [M+H] | Match by accurate mass |
| LPC(22:6) | 1.73 | 568.34 | [M+H] | MS/MS (DDA) |
| LPC(20:4) | 1.80 | 545.34 | [M+1+H] | MS/MS (DDA) |
| LPC(18:2) | 1.80 | 520.34 | [M+H] | MS/MS (DDA) |
| LPE(16:0) | 2.08 | 454.29 | [M+H] | MS/MS (DDA) |
| LPC(18:1) | 2.18 | 522.36 | [M+H] | MS/MS (DDA) |
| LPC(O-16:0) | 2.27 | 483.36 | [M+H] | MS/MS (DDA) |
| LPC(O-16:1) | 2.27 | 481.35 | [M+H] | MS/MS (DDA) |
| LPC(17:0) | 2.30 | 510.36 | [M+H] | MS/MS (DDA) |
| LPC(O-18:1) | 2.41 | 508.38 | [M+H] | MS/MS (DDA) |
| LPC(O-18:0) | 2.88 | 510.39 | [M+H] | MS/MS (DDA) |
| SM(d30:1) | 4.56 | 647.51 | [M+H] | MS/MS (DDA) |
| SM(d18:2/14:0) | 4.69 | 674.53 | [M+1+H] | MS/MS (DDA) |
| PI(16:0_16:1) | 5.05 | 549.49 | [M+H-260] | MS/MS (DDA) |
| PI(16:0_18:2) | 5.21 | 857.51 | M+Na] | MS/MS (DDA) |
| PI(16:0_20:4) | 5.22 | 859.53 | [M+H] | MS/MS (DDA) |
| SM(d18:2/16:0) | 5.45 | 723.54 | M+Na] | MS/MS (DDA) |
| PC(30:1) | 5.50 | 705.53 | [M+H] | MS/MS (DDA) |
| PI(32:0) | 5.57 | 551.50 | [M+H-260] | MS/MS (DDA) |
| PC(14:0_18:2) | 5.67 | 733.55 | [M+H+3] | MS/MS (DDA) |
| SM(d17:1/16:0) | 5.67 | 416.36 | Unassigned adduct | Match by ion coelution |
| PI(34:1) | 5.74 | 577.52 | [M+H-260] | MS/MS (DDA) |
| PC(40:8) | 5.76 | 1228.76 | Unassigned adduct | Match by ion coelution |
| PC(16:1_18:2) | 5.88 | 758.56 | [M+2+H] | MS/MS (DDA) |
| PI(18:0_20:2) | 5.91 | 863.56 | [M+H] | MS/MS (DDA) |
| PC(15:0_18:2) | 6.02 | 745.56 | [M+1+H] | MS/MS (DDA) |
| SM(d18:1/16:0) | 6.04 | 763.63 | [M+CH3CN+NH4] | MS/MS (DDA) |
| PC(42:6) | 6.07 | 844.61 | [M+H-H2O] | MS/MS (DDA) |
| PC(16:0_16:1) | 6.22 | 733.56 | [M+1+H] | MS/MS (DDA) |
| PC(16:0_22:5) | 6.33 | 1491.12 | Unassigned adduct | Match by ion coelution |
| PC(16:0_20:4) | 6.35 | 1945.41 | Unassigned adduct | Match by ion coelution |
| PC(17:0_22:6) | 6.50 | 820.58 | [M+H] | MS/MS (DDA) |
| PE(34:2) | 6.50 | 716.52 | [M+H] | MS/MS (DDA) |
| PC(18:1_18:2) | 6.58 | 1960.95 | Unassigned adduct | Match by ion coelution |
| PC(16:0_22:4) | 6.81 | 596.57 | Unassigned adduct | Match by ion coelution |
| PC(O-18:1_20:4) | 6.88 | 795.61 | [M+H] | MS/MS (DDA) |
| PC(16:0_18:1) | 6.91 | 820.63 | Unassigned adduct | Match by ion coelution |
| PC(18:0_18:2) | 7.08 | 786.75 | [M+H] | MS/MS (DDA) |
| PC(O-18:1_20:3) | 7.22 | 818.60 | M+Na] | MS/MS (DDA) |
| PC(15:0_20:1) | 7.25 | 774.60 | [M+H] | Match by accurate mass |
| PC(O-16:0_22:4) | 7.25 | 796.62 | [M+H] | Match by accurate mass |
| PC(18:0_20:3) | 7.28 | 813.62 | [M+H] | MS/MS (DDA) |
| PC(O-18:1_16:0) | 7.33 | 746.60 | [M+H] | Match by accurate mass |
| PE(O-20:0_22:6) | 7.33 | 776.56 | [M+H] | MS/MS (DDA) |
| PC(O-18:1_18:2) | 7.45 | 770.60 | [M+H] | MS/MS (DDA) |
| DG(18:1_18:2) | 7.61 | 601.52 | [M+H-H2O] | MS/MS (DDA) |
| SM(d18:2/24:1) | 7.66 | 811.67 | [M+H] | MS/MS (DDA) |
| PC(18:0_22:4) | 7.76 | 838.63 | [M+H] | MS/MS (DDA) |
| SM(d17:1/24:1) | 7.89 | 831.69 | Unassigned adduct | Match by ion coelution |
| DG(34:1) | 7.99 | 617.51 | [M+Na] | MS/MS (DDA) |
| DG(36:2) | 8.09 | 603.53 | [M+H-H2O] | MS/MS (DDA) |
| PC(O-22:1_18:1) | 8.14 | 851.67 | M+1+Na] | Match by accurate mass |
| SM(d18:1/24:1) | 8.16 | 933.64 | [M+H2PO4+Na+H] | MS/MS (DDA) |
| PC(O-20:0_20:4) | 8.16 | 826.66 | [M+H] | MS/MS (DDA) |
| PC(O-24:2_20:4) | 8.24 | 876.68 | [M+H] | Match by accurate mass |
| PC(O-24:1_20:4) | 8.72 | 879.70 | [M+1+H] | MS/MS (DDA) |
| HexCer(d18:1/24:0) | 8.91 | 812.70 | [M+H] | MS/MS (DDA) |