***Animal***

**Innate immunity and metabolomic responses in dairy cows challenged intramammarily with lipopolysaccharide after subacute ruminal acidosis**

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**Supplementary Table S1** *Ingredients and nutrient composition of the control- and the subacute rumen acidosis (SARA) diets*

|  |  |  |
| --- | --- | --- |
| Item | Control | SARA |
| Ingredients (% of dry matter) |  |  |
| Grass silage | 58.0 | 31.0 |
| Hay | 15.0 | 9.0 |
| Grain mix1 | 23.0 | 14.0 |
| Protein supplement2 | 4.0 | 0 |
| Concentrate mixture3 | 0 | 46.0 |
| Chemical composition (% of dry matter) |  |  |
| Dry matter (% of fresh feed) | 42.4 | 51.7 |
| Organic matter | 91.4 | 91.9 |
| Crude protein | 16.6 | 17.0 |
| Ether extract | 2.0 | 1.8 |
| Neutral detergent fiber | 40.9 | 33.5 |
| Non-fiber carbohydrates4 | 31.8 | 39.6 |
| Net energy of lactation (MJ/kg dry matter) | 6.66 | 7.44 |
| 1Contained: 50% corn, 47% wheat and 3% mineral and vitamin premix and consisted of (dry matter-basis): 96.7% organic matter, 11.9% crude protein, 3.2% ether extract, 14.4% neutral detergent fiber, 67.2% non-fiber carbohydrates, 8.17 MJ net energy of lactation, 2.5 g Calcium, 5.45 g Phosphorus, 7.05 g Sodium, 3.18 g Magnesium, 33,975 IU vitamin A, 5,097 IU vitamin D and 136 mg vitamin E.  2Contained: 60% rapeseed meal, 21.5% dried distillers grains with solubles, 8% soybean meal, 3% rye bran, 2.9% sugar beet molasses, 2.6% urea and 2% mineral and vitamin premix and consisted of (dry matter-basis): 92.0% organic matter, 45.5% crude protein, 3.4% ether extract, % 28.9 neutral detergent fiber, 13.9 % non-fiber carbohydrates, 7.61 MJ net energy of lactation, 10.23 g Calcium, 10.23 g Phosphorus, 3.41 g Sodium, 5.68 g Magnesium, 18 mg Copper, 80 mg Zinc, 45 mg Manganese, 1 mg Selenium, 0.6 mg Cobalt, 4 mg Iodine, 18182 IU vitamin A, 1818 IU vitamin D3 and 34 mg vitamin E.  3 Contained: 63% barley, 18% soybean meal, 9.4% rapeseed meal, 5.9% beet pulp, 2.0% mineral premix (contained 1.13% Calcium, 0.91% Phosphorus, 0.26%, Sodium, 0.50%, 13,683 IU vitamin A, 1,824 IU vitamin D, 46 mg vitamin E, 91 mg Iron, 114 mg Manganese, 68 mg Zinc and 17 mg Copper), 1.15% calcium carbonate, 0.1% salt, 0.5% monocalcium phosphate and consisted of (dry matter-basis): 93.1% organic matter, 20.8% crude protein, 2.28% ether extract, 19% neutral detergent fiber, 51% non-fiber carbohydrates, 8.62 MJ net energy of lactation. The concentrate mixture was also offered to the control cows separately at maximum of 4 kg per cow and day to reach a level of approximately 40% concentrate of the total dry matter intake.  4Non-fiber carbohydrates = (100 – (crude protein + neutral detergent fiber + ash + ether extract)). | | |

**Supplementary Table S2** *Significant correlations explaining >20% of the variation between the blood metabolomic variables and the acute phase proteins, as well as blood metabolites related to lipid and glucose metabolism and liver health measured 24 h after the lipopolysaccharide/placebo challenge. Values in the upper row present Pearson correlation coefficients, whereas values below indicate the respective P - Values*

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Amino Acids** |  |  |  |  |  | |  | | |  | | | |
| **Arginine** | Hp1 | SAA2 | LBP3 |  |  |  | |  | |
| -0.65 | -0.60 | -0.56 |  |  |  | |  | |
| <0.01 | 0.01 | 0.02 |  |  |  | |  | |
| **Asparagine** | LBP | Hp | SAA |  |  |  | |  | |
| -0.63 | -0.60 | -0.49 |  |  |  | |  | |
| 0.01 | 0.01 | 0.04 |  |  | **Correlation** | |  | |
| **Aspartate** | BHBA4 |  |  |  |  | **0.9-1.0** | | high | |
| 0.56 |  |  |  |  | **0.7-0.9** | |  | |
| 0.02 |  |  |  |  | **0.5-0.7** | |  | |
| **Citrulline** | Ca5 |  |  |  |  | **0.3-0.5** | |  | |
| 0.51 |  |  |  |  |  | | low | |
| 0.03 |  |  |  |  |  | |  | |
| **Glutamine** | Hp | SAA | LBP |  |  |  | |  | |
| -0.76 | -0.64 | -0.54 |  |  |  | |  | |
| <0.01 | <0.01 | 0.02 |  |  |  | |  | |
| **Glutamate** | BHBA | Hp |  |  |  |  | |  | |
| 0.54 | -0.48 |  |  |  |  | |  | |
| 0.02 | 0.05 |  |  |  |  | |  | |
| **Glycine** | LBP | Hp | Lactate |  |  |  | |  | |
| -0.62 | -0.47 | -0.47 |  |  |  | |  | |
| 0.01 | 0.05 | 0.05 |  |  |  | |  | |
| **Histidine** | LBP | Hp |  |  |  |  | |  | |
| -0.62 | -0.60 |  |  |  |  | |  | |
| 0.01 | 0.01 |  |  |  |  | |  | |
| **Isoleucine** | NEFA6 |  |  |  |  |  | |  | |
| -0.50 |  |  |  |  |  | |  | |
| 0.04 |  |  |  |  |  | |  | |
| **Leucine** | SAA |  |  |  |  |  | |  | |
| -0.46 |  |  |  |  |  | |  | |
| 0.05 |  |  |  |  |  | |  | |
| **Lysine** | Hp |  |  |  |  |  | |  | |
| -0.54 |  |  |  |  |  | |  | |
| 0.02 |  |  |  |  |  | |  | |
| **Phenylalanine** | GGT7 | GLDH8 | Ca |  |  |  | |  | |
| 0.67 | 0.66 | -0.56 |  |  |  | |  | |
| <0.01 | <0.01 | 0.01 |  |  |  | |  | |
| **Proline** | LBP | Hp | SAA |  |  |  | |  | |
| -0.59 | -0.57 | -0.51 |  |  |  | |  | |
| 0.01 | 0.01 | 0.03 |  |  |  | |  | |
| **Serine** | LBP | SAA | Hp |  |  |  | |  | |
| -0.67 | -0.61 | -0.58 |  |  |  | |  | |
| <0.01 | 0.01 | 0.01 |  |  |  | |  | |
| **Threonine** | Hp | LBP | SAA |  |  |  | |  | |
| -0.63 | -0.59 | -0.54 |  |  |  | |  | |
| 0.01 | 0.01 | 0.02 |  |  |  | |  | |
| **Tryptophan** | Ca |  |  |  |  |  | |  | |
| -0.49 |  |  |  |  |  | |  | |
| 0.04 |  |  |  |  |  | |  | |
| **Tyrosine** | NEFA | BHBA | Hp |  |  |  | |  | |
| -0.61 | 0.49 | -0.46 |  |  |  | |  | |
| 0.01 | 0.04 | 0.05 |  |  |  | |  | |
| **Valine** | SAA |  |  |  |  | |  | | |  | | | |
| -0.46 |  |  |  |  | |  | | |  | | | |
| 0.05 |  |  |  |  | |  | | |  | | | |
| **Biogenic Amines** | |  |  |  |  |  | | |  | | |
| **Asymmetric dimethylarginine** | GLDH | GGT | Ca |  |  |  | |  | | | | |
| -0.71 | -0.71 | 0.66 |  |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 |  |  |  | |  | | | | |
| **Creatinine** | GGT | GLDH |  |  |  |  | |  | | | | |
| 0.59 | 0.55 |  |  |  |  | |  | | | | |
| 0.01 | 0.02 |  |  |  |  | |  | | | | |
| **Dihydroxyphenylalanine** | SAA |  |  |  |  |  | |  | | | | |
| -0.57 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **Dopamine** | BHBA | Lactate |  |  |  |  | |  | | | | |
| -0.50 | 0.48 |  |  |  |  | |  | | | | |
| 0.04 | 0.04 |  |  |  |  | |  | | | | |
| **Kynurenine** | LBP | SAA |  |  |  |  | |  | | | | |
| -0.55 | -0.54 |  |  |  |  | |  | | | | |
| 0.02 | 0.02 |  |  |  |  | |  | | | | |
| **Symmetric dimehtlyarginine** | GLDH | GGT |  |  |  |  | |  | | | | |
| 0.68 | 0.67 |  |  |  |  | |  | | | | |
| <0.01 | <0.01 |  |  |  |  | |  | | | | |
| **Spermine** | GGT |  |  |  |  |  | |  | | | | |
| -0.54 |  |  |  |  |  | |  | | | | |
| 0.02 |  |  |  |  |  | |  | | | | |
| **Trans-4-Hyrdoxyproline** | Hp |  |  |  |  |  | |  | | | | |
| -0.64 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **Taurine** | GGT |  |  |  |  |  | |  | | | | |
| 0.49 |  |  |  |  |  | |  | | | | |
| 0.04 |  |  |  |  |  | |  | | | | |
| **Acylcarnitines** |  |  |  |  |  |  | |  | | | | |
| **Carnitine** | Cholesterol |  |  |  |  |  | |  | | | | |
| -0.62 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **Acetylcarnitine** | SAA | Hp |  |  |  |  | |  | | | | |
| -0.53 | -0.52 |  |  |  |  | |  | | | | |
| 0.02 | 0.03 |  |  |  |  | |  | | | | |
| **Propionylcarnitine** | NEFA | SAA |  |  |  |  | |  | | | | |
| -0.67 | -0.49 |  |  |  |  | |  | | | | |
| 0.00 | 0.04 |  |  |  |  | |  | | | | |
| **Hydroxybutyrylcarnitine** | GLDH | GGT |  |  |  |  | |  | | | | |
| 0.66 | 0.66 |  |  |  |  | |  | | | | |
| <0.01 | <0.01 |  |  |  |  | |  | | | | |
| **Hydroxypropionylcarnitine** | Ca |  |  |  |  |  | |  | | | | |
| -0.49 |  |  |  |  |  | |  | | | | |
| 0.04 |  |  |  |  |  | |  | | | | |
| **Propenoylcarnitine** | BHBA | Cholesterol |  |  |  |  | |  | | | | |
| 0.61 | 0.47 |  |  |  |  | |  | | | | |
| 0.01 | 0.05 |  |  |  |  | |  | | | | |
| **Butyrylcarnitine** | NEFA | SAA |  |  |  |  | |  | | | | |
| -0.69 | -0.47 |  |  |  |  | |  | | | | |
| <0.01 | 0.05 |  |  |  |  | |  | | | | |
| **Glutarylcarnitine** | BHBA |  |  |  |  |  | |  | | | | |
| 0.51 |  |  |  |  |  | |  | | | | |
| 0.03 |  |  |  |  |  | |  | | | | |
| **Methylglutarylcarnitine** | BHBA | Glucose |  |  |  |  | |  | | | | |
| 0.55 | 0.53 |  |  |  |  | |  | | | | |
| 0.02 | 0.02 |  |  |  |  | |  | | | | |
| **Hydroxyisovalerylcarnitine** | SAA | Hp |  |  |  |  | |  | | | | |
| -0.50 | -0.48 |  |  |  |  | |  | | | | |
| 0.04 | 0.04 |  |  |  |  | |  | | | | |
| **Octanoylcarnitine** | Glucose | LBP |  |  |  |  | |  | | | | |
| 0.53 | 0.50 |  |  |  |  | |  | | | | |
| 0.02 | 0.03 |  |  |  |  | |  | | | | |
| **Decanoylcarnitine** | LBP |  |  |  |  |  | |  | | | | |
| 0.47 |  |  |  |  |  | |  | | | | |
| 0.05 |  |  |  |  |  | |  | | | | |
| **Dodecanoylcarnitine** | Lactate |  |  |  |  |  | |  | | | | |
| 0.63 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **Tetradecanoylcarnitine** | Hp |  |  |  |  |  | |  | | | | |
| 0.46 |  |  |  |  |  | |  | | | | |
| 0.05 |  |  |  |  |  | |  | | | | |
| **Tetradecenoylcarnitine** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.74 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **Hydroxytetradecenoyl-carnitine** | Glucose |  |  |  |  |  | |  | | | | |
| 0.46 |  |  |  |  |  | |  | | | | |
| 0.05 |  |  |  |  |  | |  | | | | |
| **Hydroxytetradecadienoyl-carnitine** | NEFA | BHBA |  |  |  |  | |  | | | | |
| -0.68 | 0.47 |  |  |  |  | |  | | | | |
| <0.01 | 0.05 |  |  |  |  | |  | | | | |
| **Hexadecenoylcarnitine** | AST | Cholesterol | BHBA |  |  |  | |  | | | | |
| 0.55 | 0.52 | 0.49 |  |  |  | |  | | | | |
| 0.02 | 0.03 | 0.04 |  |  |  | |  | | | | |
| **Octadecenoylcarnitine** | GGT | GLDH |  |  |  |  | |  | | | | |
| 0.67 | 0.63 |  |  |  |  | |  | | | | |
| <0.01 | 0.01 |  |  |  |  | |  | | | | |
| **Hydroxyoctadecenoyl-**  **carnitine** | Lactate | NEFA |  |  |  |  | |  | | | | |
| 0.66 | -0.54 |  |  |  |  | |  | | | | |
| <0.01 | 0.02 |  |  |  |  | |  | | | | |
| **Phosphatidylcholines (PC)9** | |  |  |  |  |  | |  | | | | |
| **PC aa C24:0** | GLDH | GGT | AST10 |  |  |  | |  | | | | |
| 0.58 | 0.55 | 0.47 |  |  |  | |  | | | | |
| 0.01 | 0.02 | 0.05 |  |  |  | |  | | | | |
| **PC aa C26:0** | GLDH | GGT |  |  |  |  | |  | | | | |
| 0.61 | 0.58 |  |  |  |  | |  | | | | |
| 0.01 | 0.01 |  |  |  |  | |  | | | | |
| **PC aa C28:1** | NEFA | Cholesterol |  |  |  |  | |  | | | | |
| 0.63 | 0.59 |  |  |  |  | |  | | | | |
| 0.01 | 0.01 |  |  |  |  | |  | | | | |
| **PC aa C30:0** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.64 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC aa C30:2** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.60 | 0.46 |  |  |  |  | |  | | | | |
| 0.01 | 0.06 |  |  |  |  | |  | | | | |
| **PC aa C32:0** | Cholesterol | GLDH |  |  |  |  | |  | | | | |
| 0.47 | 0.46 |  |  |  |  | |  | | | | |
| 0.05 | 0.05 |  |  |  |  | |  | | | | |
| **PC aa C32:1** | GGT | GLDH | NEFA |  |  |  | |  | | | | |
| 0.70 | 0.68 | 0.50 |  |  |  | |  | | | | |
| <0.01 | <0.01 | 0.03 |  |  |  | |  | | | | |
| **PC aa C32:2** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.65 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC aa C32:3** | Cholesterol | BHBA |  |  |  |  | |  | | | | |
| 0.74 | 0.48 |  |  |  |  | |  | | | | |
| <0.01 | 0.04 |  |  |  |  | |  | | | | |
| **PC aa C34:1** | GGT | GLDH |  |  |  |  | |  | | | | |
| 0.69 | 0.69 |  |  |  |  | |  | | | | |
| <0.01 | <0.01 |  |  |  |  | |  | | | | |
| **PC aa C34:2** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.71 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC aa C34:3** | NEFA | Cholesterol |  |  |  |  | |  | | | | |
| 0.59 | 0.48 |  |  |  |  | |  | | | | |
| 0.01 | 0.05 |  |  |  |  | |  | | | | |
| **PC aa C34:4** | Cholesterol | BHBA |  |  |  |  | |  | | | | |
| 0.66 | 0.48 |  |  |  |  | |  | | | | |
| <0.01 | 0.04 |  |  |  |  | |  | | | | |
| **PC aa C36:0** | LBP |  |  |  |  |  | |  | | | | |
| 0.49 |  |  |  |  |  | |  | | | | |
| 0.04 |  |  |  |  |  | |  | | | | |
| **PC aa C36:1** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.59 | 0.47 |  |  |  |  | |  | | | | |
| 0.01 | 0.05 |  |  |  |  | |  | | | | |
| **PC aa C36:2** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.72 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC aa C36:3** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.71 | 0.49 |  |  |  |  | |  | | | | |
| <0.01 | 0.04 |  |  |  |  | |  | | | | |
| **PC aa C36:4** | Cholesterol | AST |  |  |  |  | |  | | | | |
| 0.76 | 0.47 |  |  |  |  | |  | | | | |
| <0.01 | 0.05 |  |  |  |  | |  | | | | |
| **PC aa C36:5** | Cholesterol | AST |  |  |  |  | |  | | | | |
| 0.57 | 0.49 |  |  |  |  | |  | | | | |
| 0.01 | 0.04 |  |  |  |  | |  | | | | |
| **PC aa C36:6** | Cholesterol | BHBA |  |  |  |  | |  | | | | |
| 0.54 | 0.52 |  |  |  |  | |  | | | | |
| 0.02 | 0.03 |  |  |  |  | |  | | | | |
| **PC aa C38:0** | LBP | SAA |  |  |  |  | |  | | | | |
| 0.52 | 0.47 |  |  |  |  | |  | | | | |
| 0.03 | 0.05 |  |  |  |  | |  | | | | |
| **PC aa C38:1** | GGT | GLDH |  |  |  |  | |  | | | | |
| 0.57 | 0.53 |  |  |  |  | |  | | | | |
| 0.01 | 0.02 |  |  |  |  | |  | | | | |
| **PC aa C38:3** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.56 |  |  |  |  |  | |  | | | | |
| 0.02 |  |  |  |  |  | |  | | | | |
| **PC aa C38:4** | Cholesterol | Hp |  |  |  |  | |  | | | | |
| 0.65 | 0.46 |  |  |  |  | |  | | | | |
| <0.01 | 0.05 |  |  |  |  | |  | | | | |
| **PC aa C38:5** | GLDH | AST | Cholesterol | GGT |  |  | |  | | | | |
| 0.56 | 0.54 | 0.53 | 0.50 |  |  | |  | | | | |
| 0.02 | 0.02 | 0.02 | 0.03 |  |  | |  | | | | |
| **PC aa C38:6** | Cholesterol | AST | GLDH | GGT |  |  | |  | | | | |
| 0.58 | 0.55 | 0.52 | 0.49 |  |  | |  | | | | |
| 0.01 | 0.02 | 0.03 | 0.04 |  |  | |  | | | | |
| **PC aa C40:1** | LBP |  |  |  |  |  | |  | | | | |
| 0.51 |  |  |  |  |  | |  | | | | |
| 0.03 |  |  |  |  |  | |  | | | | |
| **PC aa C40:2** | LBP | Hp | SAA |  |  |  | |  | | | | |
| 0.63 | 0.57 | 0.56 |  |  |  | |  | | | | |
| 0.01 | 0.01 | 0.02 |  |  |  | |  | | | | |
| **PC aa C40:3** | LBP | Hp | SAA |  |  |  | |  | | | | |
| 0.69 | 0.67 | 0.57 |  |  |  | |  | | | | |
| <0.01 | <0.01 | 0.01 |  |  |  | |  | | | | |
| **PC aa C40:4** | LBP | Hp | SAA |  |  |  | |  | | | | |
| 0.76 | 0.69 | 0.65 |  |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 |  |  |  | |  | | | | |
| **PC aa C40:5** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.56 |  |  |  |  |  | |  | | | | |
| 0.02 |  |  |  |  |  | |  | | | | |
| **PC aa C40:6** | AST |  |  |  |  |  | |  | | | | |
| 0.47 |  |  |  |  |  | |  | | | | |
| 0.05 |  |  |  |  |  | |  | | | | |
| **PC aa C42:0** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.47 |  |  |  |  |  | |  | | | | |
| 0.05 |  |  |  |  |  | |  | | | | |
| **PC aa C42:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.48 |  |  |  |  |  | |  | | | | |
| 0.04 |  |  |  |  |  | |  | | | | |
| **PC aa C42:2** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.70 | 0.51 |  |  |  |  | |  | | | | |
| <0.01 | 0.03 |  |  |  |  | |  | | | | |
| **PC aa C42:4** | LBP | Hp | SAA |  |  |  | |  | | | | |
| 0.82 | 0.67 | 0.57 |  |  |  | |  | | | | |
| <0.01 | <0.01 | 0.01 |  |  |  | |  | | | | |
| **PC aa C42:5** | LBP | Hp | SAA |  |  |  | |  | | | | |
| 0.65 | 0.57 | 0.52 |  |  |  | |  | | | | |
| <0.01 | 0.01 | 0.03 |  |  |  | |  | | | | |
| **PC aa C42:6** | LBP |  |  |  |  |  | |  | | | | |
| 0.48 |  |  |  |  |  | |  | | | | |
| 0.04 |  |  |  |  |  | |  | | | | |
| **PC ae C30:0** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.63 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C30:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.72 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C30:2** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.73 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C32:1** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.65 | 0.51 |  |  |  |  | |  | | | | |
| <0.01 | 0.03 |  |  |  |  | |  | | | | |
| **PC ae C32:2** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.76 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C34:0** | LBP | Hp | Cholesterol | SAA |  |  | |  | | | | |
| 0.53 | 0.51 | 0.49 | 0.46 |  |  | |  | | | | |
| 0.02 | 0.03 | 0.04 | 0.05 |  |  | |  | | | | |
| **PC ae C34:1** | GLDH | GGT | NEFA |  |  |  | |  | | | | |
| 0.54 | 0.52 | 0.50 |  |  |  | |  | | | | |
| 0.02 | 0.03 | 0.04 |  |  |  | |  | | | | |
| **PC ae C34:2** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.72 | 0.50 |  |  |  |  | |  | | | | |
| <0.01 | 0.04 |  |  |  |  | |  | | | | |
| **PC ae C34:3** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.80 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C36:1** | GLDH | GGT | Cholesterol | NEFA |  |  | |  | | | | |
| 0.51 | 0.51 | 0.49 | 0.46 |  |  | |  | | | | |
| 0.03 | 0.03 | 0.04 | 0.05 |  |  | |  | | | | |
| **PC ae C36:2** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.70 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C36:3** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.70 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C36:4** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.71 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C36:5** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.80 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C38:1** | LBP | SAA | Cholesterol |  |  |  | |  | | | | |
| 0.59 | 0.53 | 0.48 |  |  |  | |  | | | | |
| 0.01 | 0.02 | 0.04 |  |  |  | |  | | | | |
| **PC ae C38:2** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.71 | 0.49 |  |  |  |  | |  | | | | |
| <0.01 | 0.04 |  |  |  |  | |  | | | | |
| **PC ae C38:3** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.67 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C38:4** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.69 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C38:5** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.74 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C38:6** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.63 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C40:1** | LBP | Cholesterol |  |  |  |  | |  | | | | |
| 0.53 | 0.49 |  |  |  |  | |  | | | | |
| 0.03 | 0.04 |  |  |  |  | |  | | | | |
| **PC ae C40:2** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.50 | 0.49 |  |  |  |  | |  | | | | |
| 0.04 | 0.04 |  |  |  |  | |  | | | | |
| **PC ae C40:3** | Cholesterol | Glucose |  |  |  |  | |  | | | | |
| 0.66 | 0.46 |  |  |  |  | |  | | | | |
| <0.01 | 0.05 |  |  |  |  | |  | | | | |
| **PC ae C40:4** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.82 |  |  |  |  |  | |  | | | | |
| <.0001 |  |  |  |  |  | |  | | | | |
| **PC ae C40:5** | Cholesterol | AST |  |  |  |  | |  | | | | |
| 0.72 | 0.48 |  |  |  |  | |  | | | | |
| <0.01 | 0.04 |  |  |  |  | |  | | | | |
| **PC ae C40:6** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.62 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C42:0** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.64 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C42:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.73 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C42:2** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.58 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **PC ae C42:3** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.52 | 0.50 |  |  |  |  | |  | | | | |
| 0.03 | 0.04 |  |  |  |  | |  | | | | |
| **PC ae C42:4** | Cholesterol | LBP | Hp |  |  |  | |  | | | | |
| 0.67 | 0.55 | 0.49 |  |  |  | |  | | | | |
| <0.01 | 0.02 | 0.04 |  |  |  | |  | | | | |
| **PC ae C42:5** | Cholesterol | AST |  |  |  |  | |  | | | | |
| 0.76 | 0.48 |  |  |  |  | |  | | | | |
| <0.01 | 0.05 |  |  |  |  | |  | | | | |
| **PC ae C44:3** | NEFA | Cholesterol |  |  |  |  | |  | | | | |
| 0.54 | 0.46 |  |  |  |  | |  | | | | |
| 0.02 | 0.05 |  |  |  |  | |  | | | | |
| **PC ae C44:4** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.55 |  |  |  |  |  | |  | | | | |
| 0.02 |  |  |  |  |  | |  | | | | |
| **PC ae C44:5** | Cholesterol | AST | Lactate |  |  |  | |  | | | | |
| 0.55 | 0.48 | 0.47 |  |  |  | |  | | | | |
| 0.02 | 0.04 | 0.05 |  |  |  | |  | | | | |
| **PC ae C44:6** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.67 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **Sphingomyelins (SM)** |  |  |  |  |  |  | |  | | | | |
| **SM (OH) C14:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.51 |  |  |  |  |  | |  | | | | |
| 0.03 |  |  |  |  |  | |  | | | | |
| **SM (OH) C16:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.62 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **SM (OH) C22:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.51 |  |  |  |  |  | |  | | | | |
| 0.03 |  |  |  |  |  | |  | | | | |
| **SM (OH) C24:1** | Glucose |  |  |  |  |  | |  | | | | |
| 0.49 |  |  |  |  |  | |  | | | | |
| 0.04 |  |  |  |  |  | |  | | | | |
| **SM C16:0** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.68 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **SM C16:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.67 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **SM C18:0** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.67 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **SM C18:1** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.75 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **SM C20:2** | Glucose |  |  |  |  |  | |  | | | | |
| 0.53 |  |  |  |  |  | |  | | | | |
| 0.02 |  |  |  |  |  | |  | | | | |
| **SM C24:0** | LBP | SAA |  |  |  |  | |  | | | | |
| 0.47 | 0.46 |  |  |  |  | |  | | | | |
| 0.05 | 0.05 |  |  |  |  | |  | | | | |
| **SM C24:1** | Cholesterol | NEFA |  |  |  |  | |  | | | | |
| 0.54 | 0.49 |  |  |  |  | |  | | | | |
| 0.02 | 0.04 |  |  |  |  | |  | | | | |
| **SM C26:1** | Hp |  |  |  |  |  | |  | | | | |
| -0.48 |  |  |  |  |  | |  | | | | |
| 0.05 |  |  |  |  |  | |  | | | | |
| **Sum of Hexoses** | |  |  |  |  |  | |  | | | | |
| **Hexoses** | Glucose |  |  |  |  |  | |  | | | | |
| 0.65 |  |  |  |  |  | |  | | | | |
| <0.01 |  |  |  |  |  | |  | | | | |
| **Lysophosphatidylcholines (lyso PC)** | |  |  |  |  |  | |  | | | | |
| **lysoPC a C14:0** | LBP | SAA | Hp |  |  |  | |  | | | | |
| -0.84 | -0.84 | -0.69 |  |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 |  |  |  | |  | | | | |
| **lysoPC a C16:0** | SAA | LBP | Hp | Ca |  |  | |  | | | | |
| -0.82 | -0.80 | -0.75 | 0.52 |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 | 0.03 |  |  | |  | | | | |
| **lysoPC a C16:1** | LBP | SAA | Hp |  |  |  | |  | | | | |
| -0.82 | -0.77 | -0.74 |  |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 |  |  |  | |  | | | | |
| **lysoPC a C17:0** | SAA | LBP | Hp | Ca |  |  | |  | | | | |
| -0.78 | -0.75 | -0.68 | 0.54 |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 | 0.02 |  |  | |  | | | | |
| **lysoPC a C18:0** | SAA | LBP | Hp | Ca |  |  | |  | | | | |
| -0.77 | -0.73 | -0.68 | 0.52 |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 | 0.03 |  |  | |  | | | | |
| **lysoPC a C18:1** | LBP | SAA | Hp | Ca |  |  | |  | | | | |
| -0.79 | -0.78 | -0.73 | 0.49 |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 | 0.04 |  |  | |  | | | | |
| **lysoPC a C18:2** | LBP | SAA | Hp | Ca |  |  | |  | | | | |
| -0.80 | -0.80 | -0.74 | 0.49 |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 | 0.04 |  |  | |  | | | | |
| **lysoPC a C20:3** | SAA | LBP | Hp |  |  |  | |  | | | | |
| -0.77 | -0.74 | -0.68 |  |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 |  |  |  | |  | | | | |
| **lysoPC a C20:4** | SAA | LBP | Hp | Ca |  |  | |  | | | | |
| -0.76 | -0.74 | -0.70 | 0.60 |  |  | |  | | | | |
| <0.01 | <0.01 | <0.01 | 0.01 |  |  | |  | | | | |
| **lysoPC a C26:1** | NEFA |  |  |  |  |  | |  | | | | |
| 0.59 |  |  |  |  |  | |  | | | | |
| 0.01 |  |  |  |  |  | |  | | | | |
| **lysoPC a C28:0** | Cholesterol |  |  |  |  |  | |  | | | | |
| 0.55 |  |  |  |  |  | |  | | | | |
| 0.02 |  |  |  |  |  | |  | | | | |
| **lysoPC a C28:1** | Cholesterol | NEFA |  |  |  | |  | | | |  | | |
| 0.70 | 0.49 |  |  |  | |  | | | |  | | |
| <0.01 | 0.04 |  |  |  | |  | | | |  | | |

1Hp = haptoglobin.  
2SAA = serum amyloid A.  
3LBP = lipopolysaccharide-binding protein.  
4BHBA = *ß*-hydroxybutyrate.  
5Ca = calcium.  
6NEFA = non-esterified fatty acids.  
7GGT = *γ*-glutamyltransferase.  
8GLDH =glutamate dehydrogenase.  
9aa = diacyl residue; ae = acyl-alkyl residue.  
10AST = aspartate aminotransferase.