Supplementary Materials

Table S1: Means and standard deviations of relative proportions (% weight of total fatty acids) of fatty acid concentrations of human milk samples measured at 6 weeks in the Ulm Birth Cohort studies

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Fatty Acid | Common name  | SPATZ (2012)(n = 458) | UBCS (2000)(n = 567) | pvalue |
| C10:0  | Capric | 1.82 (0.51) | 2.23 (0.85) | <0.0001 |
| C12:0  | Lauric | 5.78 (1.87) | 6.50 (2.25) | <0.0001 |
| C14:0  | Myristic | 6.47 (1.58) | 7.19 (1.94) | <0.0001 |
| C16:0  | Palmitic | 23.7 (2.58) | 22.6 (2.77) | <0.0001 |
| C18:0  | Stearic | 7.27 (1.39) | 8.17 (2.19) | <0.0001 |
| C20:0  | Arachidic | 0.21 (0.04) | 0.28 (0.10) | <0.0001 |
| C22:0  | Behenic | 0.09 (0.02) | 0.16 (0.09) | <0.0001 |
| C24:0  | Lignoceric | 0.06 (0.02) | 0.16 (0.14) | <0.0001 |
| C16:1n-7  | Palmitoleic | 2.59 (0.73) | 2.78 (0.89) | 0.0004 |
| C18:1n-7  | Vaccenic | 1.76 (0.31) | 3.32 (2.81) | <0.0001 |
| C18:1n-9  | Oleic | 35.9 (3.27) | 31.1 (3.73) | <0.0001 |
| C20:1n-9  | Eicosenoic | 0.45 (0.09) | 0.38 (0.36) | <0.0001 |
| C22:1n-9  | Erucic | 0.08 (0.02) | 0.07 (0.05) | <0.0001 |
| C24:1n-9  | Nervonic | 0.07(0.03) | 0.10 (0.11) | <0.0001 |
| C16:1n-7t  |  | 0.03 (0.01) | 0.43 (0.23) | <0.0001 |
| T18:1  |  | 0.47 (0.34) | 1.12 (0.93) | <0.0001 |
| C18:2n-6tt  | Linolelaidic | 0.04 (0.05) | 0.38 (0.32) | <0.0001 |
| C18:3n-3  | α-linoleic | 0.95 (0.39) | 0.78 (0.46) | <0.0001 |
| C20:3n-3  | Dihomo-α-linolenic | 0.05 (0.01) | 0.05 (0.03) | 0.0508 |
| C20:5n-3  | Eicosapentaenoic | 0.07 (0.04) | 0.06 (0.07) | <0.0001 |
| C22:5n-3  | Docosapentanoic | 0.15 (0.04) | 0.17 (0.21) | <0.0001 |
| C22:6n-3  | Docosahexaenoic | 0.27 (0.13) | 0.23 (0.23) | <0.0001 |
| C18:2n-6  | Linoleic | 10.4 (2.68) | 10.5 (3.36) | 0.9067 |
| C18:3n-6  | γ-linolenic | 0.12 (0.04) | 0.16 (0.23) | 0.4244 |
| C20:2n-6  | Eicosadienoic | 0.28 (0.06) | 0.23 (0.09) | <0.0001 |
| C20:3n-6  | Dihomo-γ-linolenic | 0.36 (0.09) | 0.33 (0.18) | <0.0001 |
| C20:4n-6  | Arachidonic  | 0.44 (0.08) | 0.45 (0.23) | 0.1865 |
| C22:4n-6  | Adrenic | 0.09 (0.02) | 0.08 (0.08) | <0.0001 |

p values derived from Wilcoxon rank sum test comparing fatty acid concentrations measured at a 6 weeks in the SPATZ and UBCS (SPATZ versus UBCS) cohort studies. Bonferroni-adjusted level of statistical significance is α = 0.05/28 = 0.0018.

Table S2: Scoring coefficients of clr transformed fatty acids and their correlations with the identified principal components

|  |  |  |  |
| --- | --- | --- | --- |
|  Fatty Acid | Common name | PC1 | PC2 |
| C10:0  | Capric | **0.475** | 0.155 |
| C12:0  | Lauric | **0.592** | 0.329 |
| C14:0  | Myristic | **0.694** | 0.389 |
| C16:0  | Palmitic | **0.617** | **0.654** |
| C18:0  | Stearic | **0.774** | **0.400** |
| C20:0  | Arachidic | **0.761** | 0.156 |
| C22:0  | Behenic | **0.529** | -0.321 |
| C24:0  | Lignoceric | -0.026 | **-0.553** |
| C16:1n-7  | Palmitoleic | 0.390 | **0.426** |
| C18:1n-7  | Vaccenic | -0.066 | **-0.488** |
| C18:1n-9  | Oleic | 0.348 | **0.836** |
| C20:1n-9  | Eicosenoic | -0.010 | **0.477** |
| C22:1n-9  | Erucic | **-0.555** | 0.255 |
| C24:1n-9  | Nervonic | **-0.528** | -0.269 |
| C16:1n-7t  |  | **0.509** | **-0.647** |
| T18:1  |  | **0.714** | -0.002 |
| C18:2n-6tt  | Linolelaidic | **0.558** | **-0.622** |
| C18:3n-3  | α-linolenic | -0.325 | **0.484** |
| C20:3n-3  | Dihomo-α-linolenic | **-0.407** | 0.138 |
| C20:5n-3  | Eicosapentaenoic | **-0.633** | 0.122 |
| C22:5n-3  | Docosapentanoic | **-0.815** | -0.049 |
| C22:6n-3  | Docosahexaenoic | **-0.726** | 0.106 |
| C18:2n-6  | Linoleic | 0.079 | **0.603** |
| C18:3n-6  | γ-linolenic | -0.138 | 0.138 |
| C20:2n-6  | Eicosadienoic | **-0.478** | **0.576** |
| C20:3n-6  | Dihomo-γ-linolenic | **-0.529** | **0.446** |
| C20:4n-6  | Arachidonic  | **-0.643** | 0.287 |
| C22:4n-6  | Adrenic | **-0.722** | 0.037 |

Score loadings *>*0.40 or *<*−0.40 contribute to defining principal components 1 and 2 (PC1 and PC2, respectively) and are in bold.

Figure S1: Least square (LS) means scores of the two principal components retained from principal component analysis. UBCS- Ulm Birth Cohort; SPATZ- Ulm SPATZ Health Study.