**Table S5** Top 10 most notably upregulated and downregulated lipids in mature milk of different preterm and term groups (negative ion)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | EPT | FT | VIP | *P*-value | **Name** | VPT | FT | VIP | *P*-value | **Name** | MPT | FT | VIP | *P*-value |
| **Upregulated** |  |  |  |  | **Upregulated** |  |  |  |  | **Upregulated** |  |  |  |  |
| FA(18:1) | 0.70866 | 0.51798 | 1.64705 | 5.23E-08 | GlcADG(12:0/17:2) | 0.02755 | 0.00664 | 1.90786 | 7.50E-09 | GlcADG(12:0/17:2) | 0.02895 | 0.00664 | 1.81374 | 5.61E-09 |
| FA(16:2) | 0.70769 | 0.17423 | 1.87897 | 6.32E-08 | FA(16:2) | 0.60226 | 0.17423 | 1.93359 | 4.25E-08 | FAHFA(16:1/22:4) | 0.00711 | 0.00207 | 1.757 | 1.17E-07 |
| GlcADG(12:0/17:2) | 0.02729 | 0.00664 | 1.74735 | 2.48E-07 | FAHFA(18:2/14:1) | 0.00846 | 0.00097 | 1.89332 | 4.59E-07 | FA(16:2) | 0.75169 | 0.17423 | 1.8905 | 6.74E-07 |
| FAHFA(16:1/22:4) | 0.007 | 0.00207 | 1.67575 | 1.51E-06 | Cer/AS(d19:3/16:2) | 0.10244 | 0.0128 | 1.81358 | 7.13E-07 | FA(17:3) | 0.02532 | 0.00502 | 1.91929 | 1.02E-06 |
| FA(17:3) | 0.02023 | 0.00502 | 1.82093 | 2.24E-06 | FAHFA(16:1/22:4) | 0.00616 | 0.00207 | 1.79913 | 8.28E-07 | FAHFA(20:4/20:3) | 0.31046 | 0.03183 | 1.98737 | 3.98E-06 |
| FAHFA(22:3/22:4) | 0.01687 | 0.00354 | 1.69943 | 6.28E-06 | FAHFA(20:3/22:5) | 0.05209 | 0.01026 | 1.93091 | 1.35E-06 | MGDG(5:0/24:0) | 0.04139 | 0.00474 | 1.95179 | 5.24E-06 |
| FA(19:2) | 0.10731 | 0.03116 | 1.76184 | 2.96E-05 | FA(17:3) | 0.01654 | 0.00502 | 1.91319 | 1.4E-06 | FA(17:2) | 0.11079 | 0.03478 | 1.77035 | 6.47E-06 |
| FAHFA(2:0/17:2) | 0.12484 | 0.04769 | 1.68875 | 0.000101 | FA(18:1) | 0.66552 | 0.51798 | 1.44257 | 1.77E-06 | FA(18:4) | 1.24822 | 0.22967 | 1.9778 | 6.5E-06 |
| FAHFA(20:2/20:1) | 0.01762 | 0.00357 | 1.65397 | 0.000124 | FAHFA(12:0/18:2) | 0.05398 | 0.00845 | 1.82852 | 1.91E-06 | FAHFA(20:3/20:4) | 0.01179 | 0.00093 | 1.8699 | 8.69E-06 |
| FA(16:3) | 0.43768 | 0.08143 | 2.05952 | 0.000224 | FAHFA(18:1/18:2) | 0.71503 | 0.13136 | 1.80522 | 1.97E-06 | FAHFA(2:0/17:2) | 0.16244 | 0.04769 | 1.7565 | 1.27E-05 |
| **Downregulated** |  |  |  |  | **Downregulated** |  |  |  |  | **Downregulated** |  |  |  |  |
| LPE(20:0) | 0.00473 | 0.01963 | 1.65677 | 1.76E-05 | PI(18:1/18:2) | 0.04754 | 0.07016 | 1.48146 | 6.65E-05 | PI(18:1/18:2) | 0.04154 | 0.07016 | 1.53883 | 2.65E-06 |
| HexCer/AP(t16:2/20:1) | 0.00183 | 0.00987 | 1.6154 | 3.72E-05 | OxPS(18:0/20:3+4O(1Cyc)) | 0.00973 | 0.01455 | 1.72661 | 8.25E-05 | OxPS(18:0/20:3+4O(1Cyc)) | 0.00855 | 0.01455 | 1.73566 | 3.57E-06 |
| LPE(22:2) | 0.00564 | 0.03691 | 1.53937 | 5.90E-05 | SQDG(21:2/22:6) | 0.00722 | 0.00973 | 1.2723 | 0.000146 | PE(18:2/20:2) | 0.00295 | 0.00682 | 1.22671 | 1.69E-05 |
| LPE(22:4) | 0.019 | 0.09987 | 1.60419 | 8.29E-05 | LPC(18:0) | 0.06963 | 0.10971 | 1.1036 | 0.000149 | PC(18:1/20:4) | 0.00404 | 0.00864 | 1.29444 | 2.27E-05 |
| LPS(22:6) | 0.00257 | 0.01445 | 1.65945 | 8.89E-05 | PC(18:1/20:4) | 0.00459 | 0.00864 | 1.33562 | 0.000173 | PE(18:1/18:1) | 0.02021 | 0.03545 | 1.21053 | 6.87E-05 |
| HexCer/AP(t14:1/22:2) | 3.74E-05 | 0.00058 | 1.56567 | 0.000105 | LPE(18:0) | 0.00483 | 0.01225 | 1.13276 | 0.000370 | PE(18:0/20:5) | 0.01875 | 0.05097 | 1.22495 | 6.88E-05 |
| LPE(18:0) | 0.00403 | 0.01225 | 1.46263 | 0.000112 | PC(18:1/18:1) | 0.01361 | 0.02208 | 1.60035 | 0.000532 | LPC(18:0) | 0.06164 | 0.10971 | 1.30382 | 7.50E-05 |
| PI(18:1/18:2) | 0.03804 | 0.07016 | 1.75584 | 0.000118 | PE(18:1/18:1) | 0.02264 | 0.03544 | 1.50898 | 0.000617 | PI(18:1/20:3) | 0.00337 | 0.00566 | 1.07553 | 0.000233 |
| LPE(20:1) | 0.07903 | 0.19836 | 1.38609 | 0.000141 | HBMP(14:0/14:1/14:1) | 0.12541 | 0.16141 | 1.09317 | 0.000699 | PC(18:1/18:1) | 0.01319 | 0.02208 | 1.51971 | 0.000245 |
| LPS(18:0) | 0.01055 | 0.02726 | 1.39393 | 0.000161 | LPE(18:1) | 0.14778 | 0.31663 | 1.28895 | 0.000704 | SQDG(21:2/22:6) | 0.00736 | 0.00973 | 1.13339 | 0.00031 |

EPT: extremely preterm; VPT: very preterm; MPT: moderately preterm; FT: full-term; VIP: variable importance in projection of the OPLS-DA model.