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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Supplementary Table 1.** Relationships between twin, diamniotic, dichorionic pregnancy (vs. singleton pregnancy) and relevant parameters (with significant variable importance, p<0.05) in serum from umbilical artery at labour as evaluated by OPLS and ordinary multiple regression (OMR) models (for details see Statistical analysis) | | | | | | | | | | | | |
|  |  | **OPLS, predictive component** | | | | | | |  | **Multiple**  **regression** | | |
|  | **Variable** | Variable importance | t-statistics | | Component loading | t-statistics | R*a* | |  | Regression coefficient | t-statistics | |
| EXPLAINING VARIABLES | Gestational age | 1.21 | 5.02 | \*\* | -0.190 | -6.29 | -0.584 | \*\* |  | -0.102 | -3.52 | \*\* |
| Pregnenolone | 0.918 | 3.38 | \*\* | 0.162 | 3.55 | 0.500 | \*\* |  | 0.077 | 2.93 | \* |
| Pregnenolone, C | 1.032 | 2.38 | \* | -0.187 | -2.51 | -0.577 | \* |  | -0.099 | -3.49 | \*\* |
| 16α-Hydroxypregnenolone | 1.225 | 3.88 | \*\* | 0.211 | 3.89 | 0.648 | \*\* |  | 0.054 | 1.64 |  |
| 20α-Dihydropregnenolone | 1.27 | 4.14 | \*\* | 0.209 | 5.04 | 0.644 | \*\* |  | 0.091 | 3.43 | \*\* |
| Dehydroepiandrosterone, C | 0.994 | 3.67 | \*\* | -0.182 | -4.07 | -0.562 | \*\* |  | -0.098 | -5.25 | \*\* |
| 7-oxo-DHEA | 0.86 | 3.08 | \*\* | 0.135 | 3.08 | 0.409 | \*\* |  | 0.010 | 0.29 |  |
| Androstenediol, C | 0.62 | 2.51 | \* | -0.107 | -3.50 | -0.331 | \*\* |  | -0.027 | -0.88 |  |
| 17-Hydroxyprogesterone | 0.455 | 2.52 | \* | 0.065 | 1.94 | 0.200 | \* |  | 0.016 | 0.57 |  |
| 17,20α-Dihydroxy-4-pregnene-3-one | 0.623 | 2.26 | \* | 0.084 | 2.00 | 0.257 | \* |  | 0.017 | 0.54 |  |
| 20α-Dihydroprogesterone | 0.945 | 3.02 | \*\* | 0.175 | 4.00 | 0.536 | \*\* |  | 0.004 | 0.14 |  |
| Estradiol, C | 0.852 | 2.75 | \* | 0.173 | 2.95 | 0.539 | \* |  | 0.022 | 0.68 |  |
| 5α-Dihydroprogesterone | 1.248 | 4.70 | \*\* | 0.207 | 5.55 | 0.634 | \*\* |  | 0.051 | 1.27 |  |
| Allopregnanolone | 1.131 | 9.26 | \*\* | 0.200 | 6.40 | 0.614 | \*\* |  | 0.035 | 2.40 | \* |
| Allopregnanolone, C | 0.662 | 2.04 | \* | 0.114 | 2.30 | 0.359 | \* |  | -0.009 | -0.40 |  |
| Isopregnanolone | 1.511 | 12.29 | \*\* | 0.260 | 23.47 | 0.798 | \*\* |  | 0.063 | 2.98 | \* |
| 5α,20α-Tetrahydroprogesterone | 1.309 | 7.94 | \*\* | 0.235 | 7.49 | 0.722 | \*\* |  | 0.034 | 2.15 | \* |
| 5α-Pregnane-3α,20α-diol | 1.267 | 8.12 | \*\* | 0.218 | 6.34 | 0.669 | \*\* |  | 0.049 | 3.66 | \*\* |
| 5α-Pregnane-3α,20α-diol, C | 0.791 | 2.49 | \* | 0.144 | 2.79 | 0.449 | \* |  | 0.019 | 0.73 |  |
| 5α-Pregnane-3β,20α-diol | 1.525 | 9.48 | \*\* | 0.275 | 10.89 | 0.844 | \*\* |  | 0.063 | 2.91 | \* |
| 5α-Pregnane-3β,20α-diol, C | 0.907 | 3.29 | \*\* | 0.152 | 3.18 | 0.475 | \*\* |  | 0.023 | 1.14 |  |
| 17-Hydroxyallopregnanolone | 0.854 | 3.48 | \*\* | 0.147 | 3.67 | 0.450 | \*\* |  | 0.011 | 0.45 |  |
| 17-Hydroxyallopregnanolone, C | 0.506 | 2.58 | \* | 0.078 | 2.33 | 0.236 | \* |  | -0.031 | -2.09 | \* |
| 17-Hydroxypregnanolone | 0.678 | 2.88 | \* | 0.093 | 2.93 | 0.283 | \* |  | 0.021 | 0.54 |  |
| 17-Hydroxypregnanolone, C | 0.812 | 2.97 | \* | 0.110 | 1.87 | 0.339 |  |  | 0.028 | 1.47 |  |
| 5α-Pregnane-3α,17,20α-triol | 0.678 | 2.54 | \* | 0.075 | 1.54 | 0.229 |  |  | 0.024 | 1.25 |  |
| Androsterone, C | 0.793 | 1.95 | \* | -0.158 | -2.27 | -0.486 | \* |  | -0.094 | -4.03 | \*\* |
| 5α-Androstane-3α,17β-diol | 0.777 | 1.95 | \* | 0.114 | 1.46 | 0.345 |  |  | 0.042 | 1.62 |  |
| 5α-Androstane-3α,17β-diol, C | 0.709 | 2.03 | \* | 0.094 | 1.42 | 0.295 |  |  | 0.020 | 0.70 |  |
| Corticosterone | 0.662 | 2.77 | \* | 0.089 | 1.87 | 0.271 |  |  | 0.012 | 0.54 |  |
| 21-Deoxycortisol | 1.138 | 4.36 | \*\* | 0.175 | 4.05 | 0.537 | \*\* |  | 0.047 | 1.97 | \* |
| 11-Deoxycorticosterone | 0.897 | 4.06 | \*\* | 0.144 | 3.59 | 0.441 | \*\* |  | 0.037 | 1.53 |  |
| 11β-Hydroxytestosterone, C | 1.161 | 3.06 | \*\* | -0.175 | -2.47 | -0.539 | \* |  | -0.101 | -3.09 | \*\* |
| 3α,5β-Tetrahydrocorticosterone | 1.796 | 11.82 | \*\* | 0.291 | 13.01 | 0.906 | \*\* |  | 0.117 | 5.94 | \*\* |
| 11β-Hydroxyepiandrosterone | 0.625 | 2.63 | \* | 0.125 | 3.38 | 0.379 | \*\* |  | -0.023 | -1.03 |  |
| 11β-Hydroxyepiandrosterone, C | 0.855 | 3.20 | \*\* | 0.109 | 2.10 | 0.351 | \* |  | 0.046 | 1.27 |  |
|  | Twins (diamniotic dichorionic) |  |  |  | 1.000 | 25.93 | 0.862 | \*\* |  |  | | |
| Explained variability = 74.3% (63.1% after cross-validation), Sensitivity = 0.962(0.888-1), Specificity = 1(1-1) | | | | | | | | | | | | |
| *aR…Component loading expressed as a correlation coefficient with predictive component, \*p<0.05, \*\*p<0.01, LLR…logarithm of likelihood ratio (the ratio of the probability that the phenomenon occurs - twin pregnancy) to the probability that the phenomenon does not occur - singleton pregnancy), C…conjugated steroid* | | | | | | | | | | | | |