**Animal journal. Salivary and urinary metabolome analysis for pre-puberty-related biomarkers identification in porcine.**

Ghylène Goudet, Lydie Nadal-Desbarats, Cécile Douet, Jonathan Savoie, Christophe Staub, Eric Venturi, Stéphane Ferchaud, Sylviane Boulot, Armelle Prunier

**Supplementary Table S1** *Summary of the quality criteria of the Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) models fitted on porcine urine data*

|  |  |  |  |
| --- | --- | --- | --- |
| OPLS-DA model | Quality of the models | | |
| *R²*Y(cum) | *Q²*(cum) | CV-ANOVA |
| week-5 *versus* -4 | 0.66 | 0.22 | 0.33 |
| week-5 *versus* -3 | 0.97 | 0.845 | 0.02 |
| week-5 *versus* -2 | No model | | |
| week-5 *versus* -1 | 0.73 | 0.14 | 0.89 |
| week-4 *versus* -3 | No model | | |
| week-4 *versus* -2 | 0.95 | 0.85 | 0.005 |
| week-4 *versus* -1 | 0.58 | 0.42 | 0.11 |
| week-3 *versus* -2 | 0.88 | 0.18 | 0.80 |
| week-3 *versus* -1 | 0.78 | 0.475 | 0.35 |
| week-2 *versus* -1 | 0.67 | 0.31 | 0.23 |

**Supplementary Table S2** *Porcine urine metabolites identified by Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) discriminating week-5 versus week-3 before puberty.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Var ID (Metabolites) | VIP | *P*-value | Fold Change ratio  (week-3/ week-5) | -3/-5 |
| Und-1.61 | 1.77 | 0.0012 | 0.75 | Down |
| Alanine | 1.51 | 0.011 | 0.84 | Down |
| Und-1.57 | 1.52 | 0.012 | 0.76 | Down |
| (Pyruvate+X) | 1.39 | 0.04 | 0.80 | Down |
| Und-0.93 | 1.35 | 0.03 | 0.86 | Down |
| Lactate | 1.30 | 0.04 | 0.84 | Down |
| DimethylSulfone | 1.30 | 0.04 | 1.27 | Up |
| Und-3.36 | 1.29 | 0.04 | 1.22 | Up |
| IsovalerylGlycine | 1.07 | 0.17 | 0.88 | Down |
| Trigonelline | 1.07 | 0.12 | 1.27 | Up |
| Glycine | 1.01 | 0.18 | 0.77 | Down |
| Tyrosine+*p*Cresol | 0.96 | 0.14 | 0.86 | Down |
| VIP = variable Importance in Projection in the OPLS-DA model. *P*-value obtained by a non-parametric test (Wilcoxon rank-sum test). Und = undetermined, X: unknown | | | | |

**Supplementary Table S3** *Summary of the quality criteria of the Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) models fitted on porcine saliva data.*

|  |  |  |  |
| --- | --- | --- | --- |
| OPLS-DA model | Quality of the models | | |
| *R²*Y(cum) | *Q²*(cum) | CV-ANOVA |
| Week-5 *versus* -4 | No model | | |
| week-5 *versus* -3 | 0.64 | 0.5 | 0.24 |
| week-5 *versus* -2 | 0.45 | 0.22 | 0.74 |
| week-5 *versus* -1 | 0.64 | 0.48 | 0.27 |
| week-4 *versus* -3 | No model | | |
| week-4 *versus* -2 | No model | | |
| week-4 *versus* -1 | 0.92 | 0.75 | 0.07 |
| week-3 *versus* -2 | No model | | |
| week-3 *versus* -1 | 0.74 | 0.51 | 0.22 |
| week-2 *versus* -1 | 0.25 | 0.16 | 0.45 |

**Supplementary Table S4** *Porcine* s*aliva metabolites identified by Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) discriminating week-4 versus week-1 before puberty.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Var ID (Metabolites) | VIP | *P*-value | Fold Change ratio  (week-1/ week-4) | -1/-4 |
| Malonate | 1.51 | 0.004 | 1.62 | Up |
| Und-4.59 | 1.21 | 0.06 | 1.81 | Up |
| Und-5.79 | 1.18 | 0.09 | 1.58 | Up |
| Ethanol | 1.168 | 0.025 | 1.80 | Up |
| Butyrate-2-HOvalerate | 1.09 | 0.13 | 1.80 | Up |
| Und-0.85 | 0.95 | 0.13 | 1.74 | Up |
| VIP = variable Importance in Projection in the OPLS-DA model. *P*-value obtained by a non-parametric test (Wilcoxon rank-sum test). Und = undetermined. | | | | |

**Supplementary Table S5**  *porcine saliva metabolites identified by Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) discriminating week-5 versus week-1 before puberty.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Var ID (Metabolites) | VIP | *P*-value | Fold Change ratio  (week-1/ week-5) | -1/-5 |
| Und-5.79 | 1.30 | 0.03 | 1.70 | Up |
| Propionate | 1.30 | 0.08 | 1.50 | Up |
| Ethanol | 1.22 | 0.12 | 1.65 | Up |
| Malonate | 1.18 | 0.12 | 1.35 | Up |
| Butyrate+2HOvalerate | 1.15 | 0.05 | 1.67 | Up |
| Formate | 1.10 | 0.17 | 1.67 | Up |
| VIP = variable Importance in Projection in the OPLS-Da model. *P*-value obtained by a non-parametric test (Wilcoxon rank-sum test). Und = undetermined. | | | | |