

Supplementary SA. Figures

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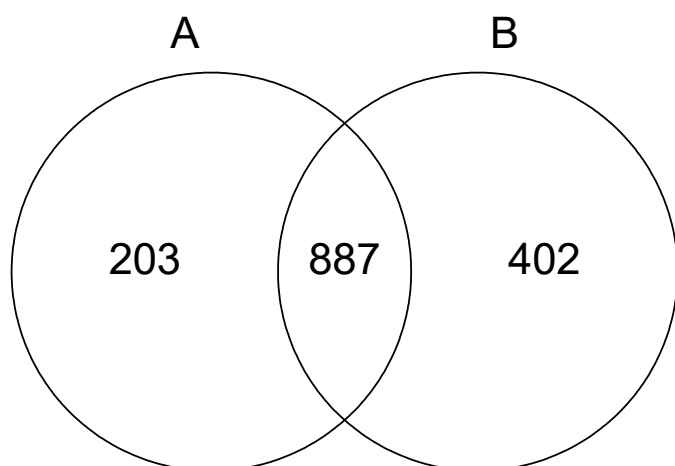


Figure SA1. Venn diagram from the two tested algorithms; “baseline cut-off” (A) and “Wavelets” (B) 887 common features are in the common section.

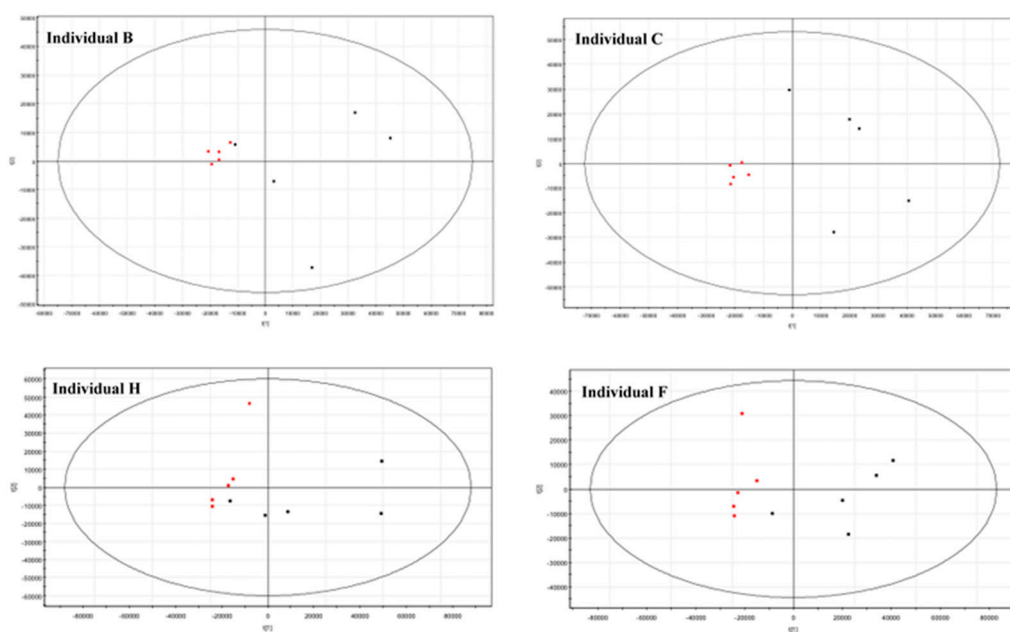


Figure SA2. PCA scores plots of representative individuals’ (B, C, H and F) urine samples (P and O) after UV scaling, obtained from UHPLC-(+)ESI-HRMS analysis. A clear trend towards the differentiation between P (red) and O (black) samples was observed in each individual separately.

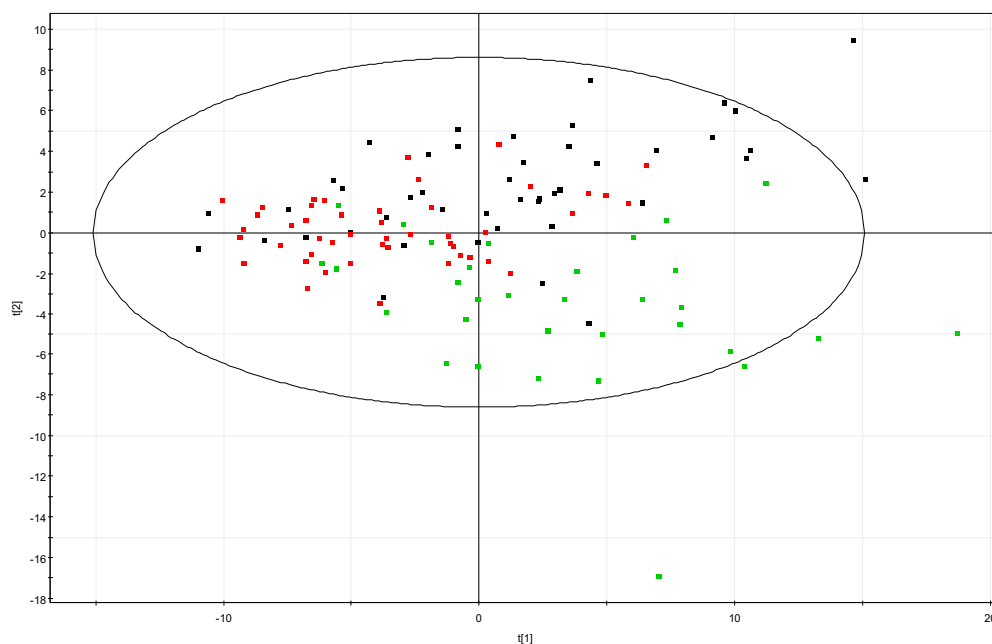


Figure SA3. PLS-DA scores plot (UV scaled) of B, P and O urine samples from all the days of the administration, obtained by UHPLC-(+)ESI-HRMS. No significant clustering was observed between the B samples (green points) the O samples (black points) and the P samples (red points).

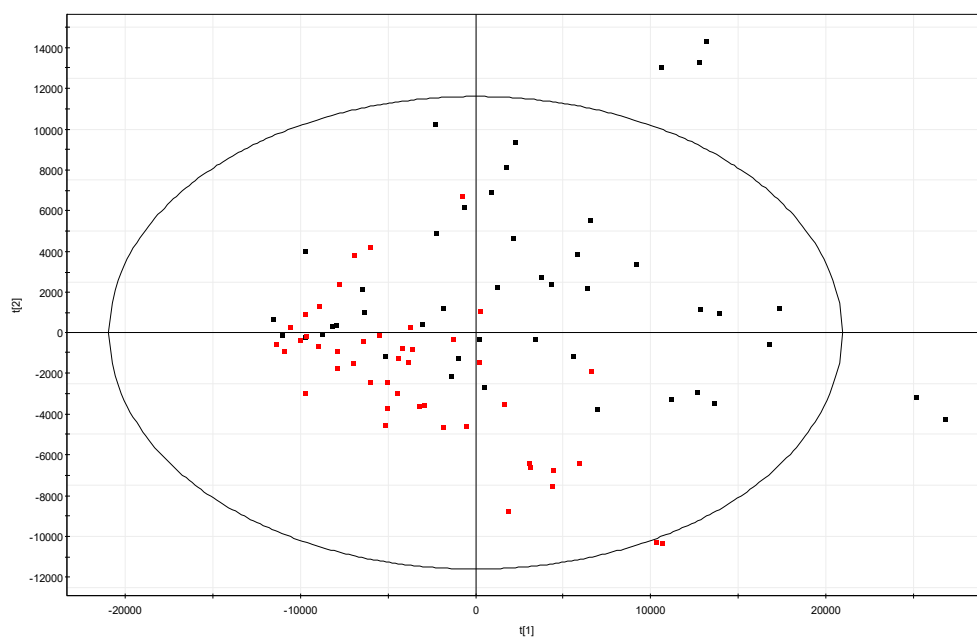


Figure SA4. PLS-DA scores plot (UV scaled) of P and O urine samples from all the days of the administration, obtained by UHPLC-(+)ESI-HRMS. No significant clustering was observed between the O samples (black points) and the P samples (red points).

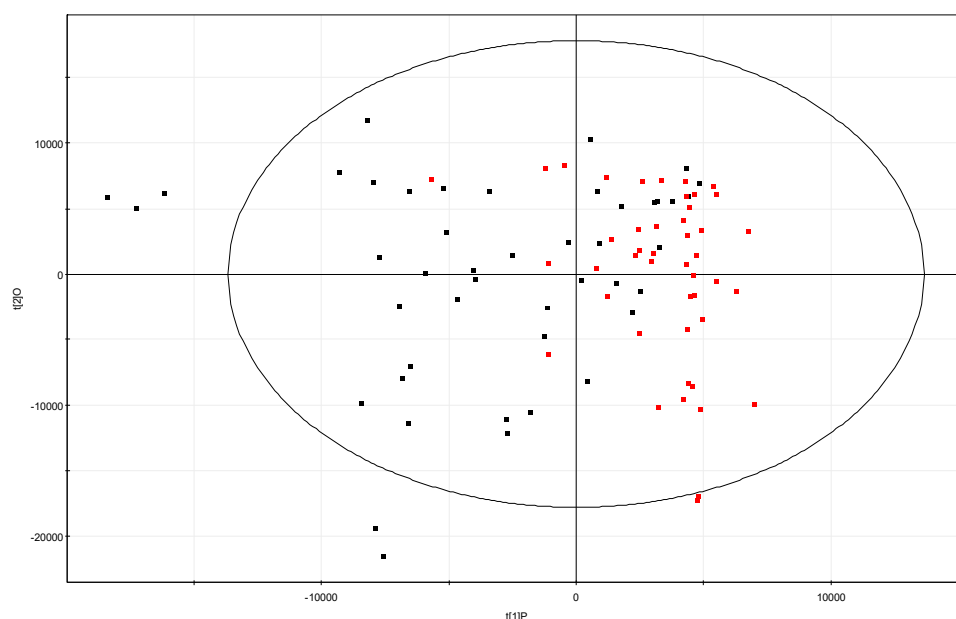


Figure SA5. OPLS-DA scores plot (UV scaled) of P and O urine samples from all the days of the administration, obtained by UHPLC-(+)ESI-HRMS. No significant clustering was observed between the O samples (black points) and the P samples (red points), even if they have the tendency to form two separate classes/groups.

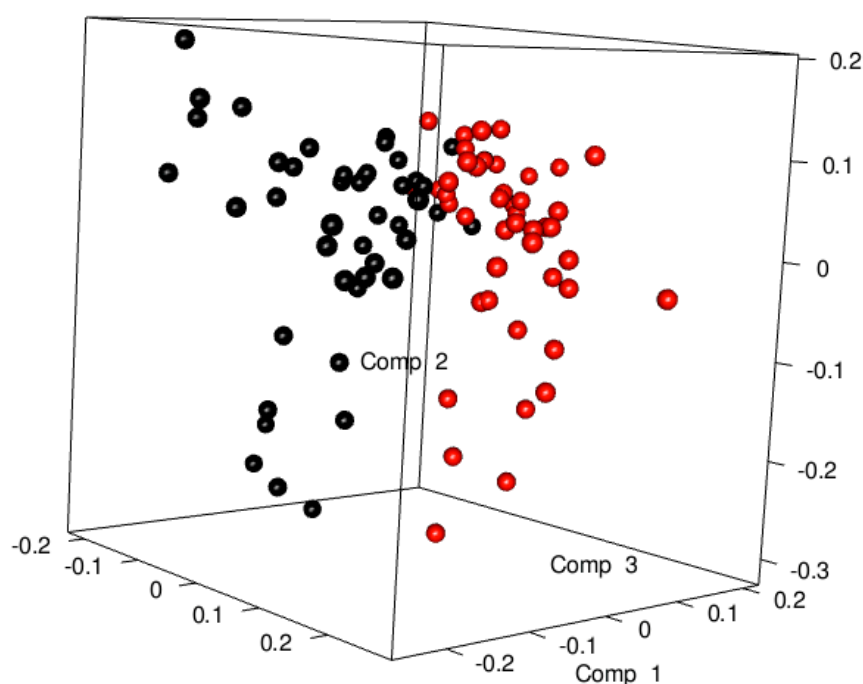


Figure SA6. 2-level ML-PLS-DA analysis of the P and O urine samples from all the days of administration, obtained by UHPLC-(+)ESI-HRMS. The 3-D multilevel PLS-DA scores plot (Comp 1, Comp 2, Comp 3) of the combination of the within subject variation and the day-based effect ($\text{Var}_{\text{within}} + \text{Var}_{\text{day}}$) with the biological variation ($\text{Var}_{\text{between}}$) being subtracted is shown. Red circles represent the P samples. Black circles represent the O samples. A clear clustering between P and O samples, is shown.