Supplementary Information to:

Metabolic fingerprint after acute and under sustained consumption of a functional beverage based on grape skin extract in healthy human subjects

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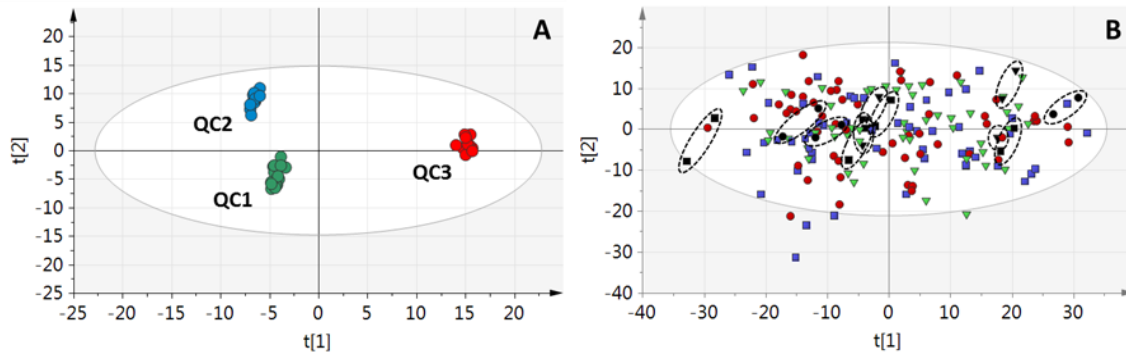
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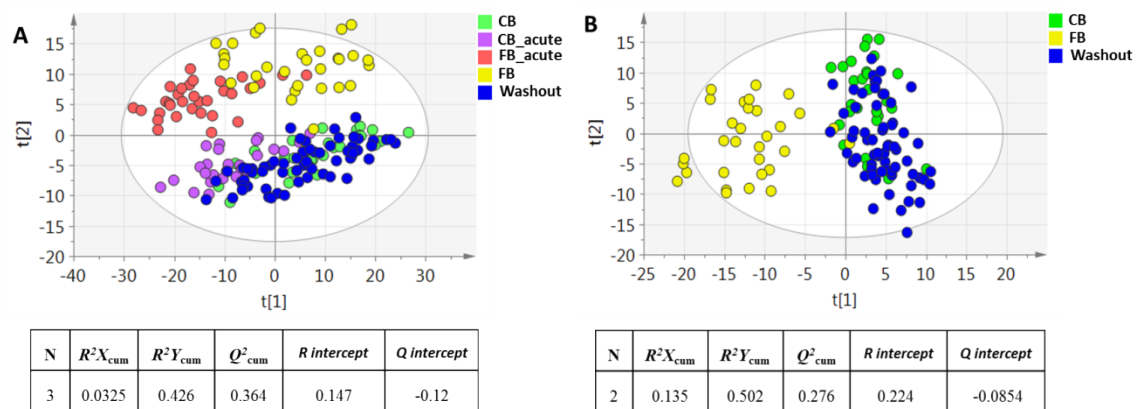Rafael Llorach Tel.: +34 934033798; fax: +34 934035931. *E-mail address*:

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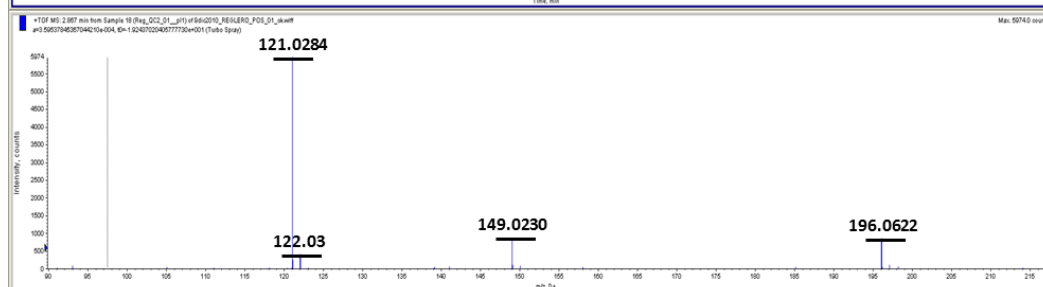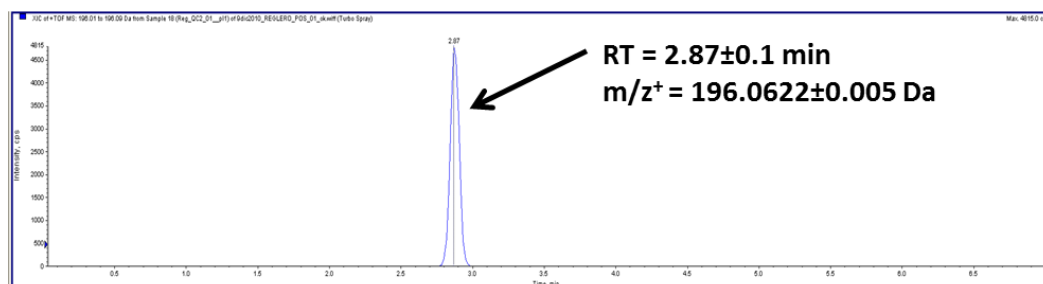
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Figure 1S (Supplementary Information): (A) PCA scores plot of samples belonging to quality controls: QC1, QC2 and QC3; **(B)** PCA scores plot of urine samples belonging to the acute and sustained interventions and to the QC4. Coloured symbols indicate the 3 injected batches: blue squares (batch 1), red circles (batch 2) and green triangles (batch 3), whereas black symbols surrounded by dashed lines in circles are re-injected within the same batch samples (QC4).
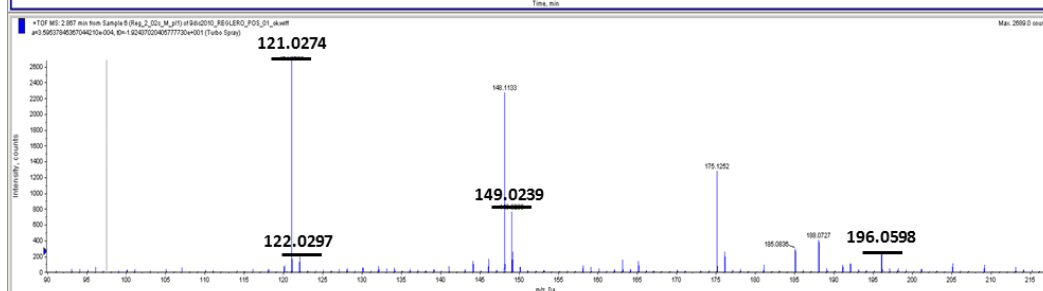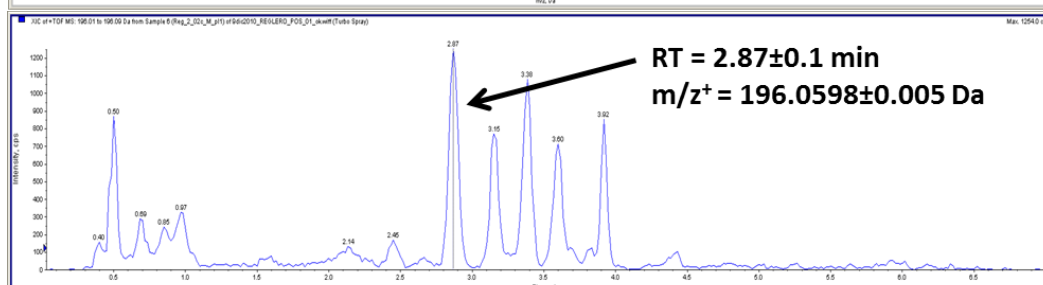

N	R^2X_{cum}	R^2Y_{cum}	Q^2_{cum}	R intercept	Q intercept
3	0.0325	0.426	0.364	0.147	-0.12

N	R^2X_{cum}	R^2Y_{cum}	Q^2_{cum}	R intercept	Q intercept
2	0.135	0.502	0.276	0.224	-0.0854

Figure 2S (Supplementary Information): Scores plots deriving from PLS-DA model built using metabolome data from: **(A)** urine samples collected before (blue circles correspond to washout), after acute (red and green circles correspond to functional (FB) and control (CB) beverage consumption, respectively) and under sustained (yellow and violet circles correspond to functional and control beverage consumption, respectively); and **(B)** 24-hour urine samples collected before (blue circles correspond to washout) and under sustained (yellow and green circles correspond to functional (FB) and control (CB) beverage consumption, respectively) intervention with tested drinks. N – number of components in PLS-DA modelling; R^2X_{cum} and R^2Y_{cum} are the cumulative modelled variations in the X and Y matrix, respectively; Q^2_{cum} – the cumulative predicted variation in the Y matrix; R and Q intercepts are obtained from 200 permutation tests of both PLS-DA models.

Figure 3S (Supplementary Information): Extracted ion chromatogram and mass spectrum of the standard from QC 2 and identified in urine 4-hydroxyhippuric acid. Assignations for generated in-source fragments of 4-hydroxyhippuric acid are present within Table 1.