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Metabolomic approach determine exposure to bioactive compounds after consumption of tropical highland blackberry (Rubus adenotrichus) juice

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INTRODUCTION

Consumption of polyphenol-rich foods continues to be the focus of attention because of their putative impact on human health. Tropical highland blackberry (Rubus adenotrichus) juice is widely consumed from Mexico to Ecuador and represents an important source of ellagitannins and others phytochemicals for the population. Using blackberry as a model for other tropical fruits, we have shown how metabolomic profiling can be used to characterize individual exposure to bioactive molecules and their metabolites in a nutritional trial on healthy volunteers.

NUTRITIONAL STUDY DESIGN

Fourteen Costa Rican men consumed for 8 days a daily dose of 250mL of a locally produced and well characterized blackberry juice, as part of a controlled diet.

24hr urines collected before and at the end of the supplementation were analyzed with a non-targeted high-resolution mass spectrometry (UPLC-QqToF) method.

ANALYSIS

After pre-processing of LC-QqToF data, statistical analyses were applied:
- ANOVA (R)
- PCA and OSC-PLS-DA on log-pareto data (SIMCA 13.0)

RESULTS

1919 ions were detected (ESI+) in the profiles, of which 226 had statistically a different intensity (ANOVA) in the two groups

IDENTIFICATION OF THE UROLITHINS AS MAJOR DISCRIMINANTS IONS

The mass spectra of the discriminant ions show the parent ions, in both cases mono-glucuronide derivatives, as well as correlated fragments and adducts. The major ion in both cases corresponds to the in-source fragmentation into aglycone. The chromatograms of the aglycone fragments at Rt 9.78 and 10.92 for UA and UB respectively, show the marked intensity increase after blackberry juice consumption.

CONCLUSION

The metabolomic analysis discriminated the consumption of blackberry juice by the volunteers with more than 60 strong discriminants. Interestingly, the microbial metabolites of urolithins, urolitin A-glucuronide and urolitin B-glucuronide, were the most important discriminants but other ions currently under identification could also contribute to blackberry juice health effects. Correlations will be searched between all discriminant metabolites and the individual capacity to produce UA and UB to further investigate inter individual variation in response to blackberry juice intake.