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Metabolomic approach determine exposure to bioactive compounds after consumption of tropical highland blackberry (Rubus adnoretichus) 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 adnoretichus) juice is widely consumed from Mexico to Ecuador and represents an important source of ellagitanins 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-QToF) method.

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

ANALYSIS

List of discriminant ions:

Blackberry’s metabolite database creation: Compounds of blackberry composition data
- In silico prediction of blackberry phytochemical metabolites and MS/MS fragmentation
- Online databases

RESULTS

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

We identified three types of subjects: the producers of urolithin A (A), the producers of urolithin B (B) and the weak urolithins producers (N) after consumption of blackberry juice (purple columns). (Blue columns correspond to consumption of water)

CONCLUSION

The metabolic analysis discriminated the consumption of blackberry juice by the volunteers with more than 60 strong discriminants. Interestingly, the microbial metabolites of urolithins, urolithin A-glucuronide and urolithin 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.