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**Metabolomic approach determine exposure to bioactive compounds after consumption of tropical highland blackberry (Rubus adnestrichus) 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 adnestrichus) juice is widely consumed from Mexico to Ecuador and represents an important source of ellagitannins and other 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**

Blackberry's metabolite database creation: Compilation of blackberry composition data

+ In silico prediction of blackberry phytochemical metabolism and MS/MS fragmentation

**RESULTS**

**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 source fragmentation into aglycone. The chromatograms of the aglycone fragments at RT 9.78 and 9.84 for UA and UB respectively, show the marked intensity increase after blackberry juice consumption.

**CHARACTERIZATION OF VOLUNTEERS**

The urine metabolome analyzed before (blue) and after (purple) blackberry juice were clearly distinguished by PLS-DA (figure A) with a good validation of the model (Q2cum = 0.674, permutation test r = 100). The loading plot shows all detected ions. Red points correspond to VIP higher than 2 and green points correspond to VIP higher than 1.5 (figure B). The identification of the other strong discriminants is in progress [analysis using ultra-high resolution M/ELTQOrbitrap]

**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, 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.