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

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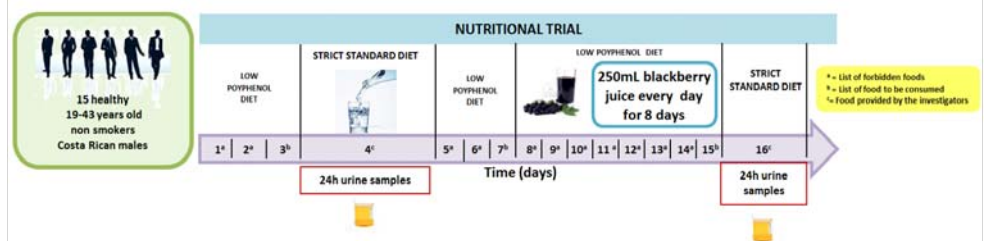
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INTRODUCTION

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.

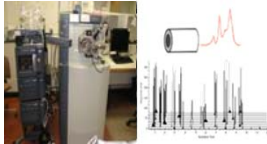
NUTRITIONAL STUDY DESIGN

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.



ANALYSIS

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)

List of discriminant ions: Identification

Ion	Formula	Retention Time (min)	Abundance	Identification
145.022	C ₁₀ H ₁₁ O ₃	10.9	100	Urolithin A
161.037	C ₁₁ H ₁₃ O ₃	10.9	100	Urolithin B
177.052	C ₁₂ H ₁₅ O ₃	10.9	100	Urolithin A glucuronide
193.067	C ₁₃ H ₁₇ O ₃	10.9	100	Urolithin B glucuronide
209.082	C ₁₄ H ₁₉ O ₃	10.9	100	Urolithin A glucuronide
225.097	C ₁₅ H ₂₁ O ₃	10.9	100	Urolithin B glucuronide
241.112	C ₁₆ H ₂₃ O ₃	10.9	100	Urolithin A glucuronide
257.127	C ₁₇ H ₂₅ O ₃	10.9	100	Urolithin B glucuronide
273.142	C ₁₈ H ₂₇ O ₃	10.9	100	Urolithin A glucuronide
289.157	C ₁₉ H ₂₉ O ₃	10.9	100	Urolithin B glucuronide
305.172	C ₂₀ H ₃₁ O ₃	10.9	100	Urolithin A glucuronide
321.187	C ₂₁ H ₃₃ O ₃	10.9	100	Urolithin B glucuronide
337.202	C ₂₂ H ₃₅ O ₃	10.9	100	Urolithin A glucuronide
353.217	C ₂₃ H ₃₇ O ₃	10.9	100	Urolithin B glucuronide
369.232	C ₂₄ H ₃₉ O ₃	10.9	100	Urolithin A glucuronide
385.247	C ₂₅ H ₄₁ O ₃	10.9	100	Urolithin B glucuronide
401.262	C ₂₆ H ₄₃ O ₃	10.9	100	Urolithin A glucuronide
417.277	C ₂₇ H ₄₅ O ₃	10.9	100	Urolithin B glucuronide
433.292	C ₂₈ H ₄₇ O ₃	10.9	100	Urolithin A glucuronide
449.307	C ₂₉ H ₄₉ O ₃	10.9	100	Urolithin B glucuronide
465.322	C ₃₀ H ₅₁ O ₃	10.9	100	Urolithin A glucuronide
481.337	C ₃₁ H ₅₃ O ₃	10.9	100	Urolithin B glucuronide
497.352	C ₃₂ H ₅₅ O ₃	10.9	100	Urolithin A glucuronide
513.367	C ₃₃ H ₅₇ O ₃	10.9	100	Urolithin B glucuronide
529.382	C ₃₄ H ₅₉ O ₃	10.9	100	Urolithin A glucuronide
545.397	C ₃₅ H ₆₁ O ₃	10.9	100	Urolithin B glucuronide
561.412	C ₃₆ H ₆₃ O ₃	10.9	100	Urolithin A glucuronide
577.427	C ₃₇ H ₆₅ O ₃	10.9	100	Urolithin B glucuronide
593.442	C ₃₈ H ₆₇ O ₃	10.9	100	Urolithin A glucuronide
609.457	C ₃₉ H ₆₉ O ₃	10.9	100	Urolithin B glucuronide
625.472	C ₄₀ H ₇₁ O ₃	10.9	100	Urolithin A glucuronide
641.487	C ₄₁ H ₇₃ O ₃	10.9	100	Urolithin B glucuronide
657.502	C ₄₂ H ₇₅ O ₃	10.9	100	Urolithin A glucuronide
673.517	C ₄₃ H ₇₇ O ₃	10.9	100	Urolithin B glucuronide
689.532	C ₄₄ H ₇₉ O ₃	10.9	100	Urolithin A glucuronide
705.547	C ₄₅ H ₈₁ O ₃	10.9	100	Urolithin B glucuronide
721.562	C ₄₆ H ₈₃ O ₃	10.9	100	Urolithin A glucuronide
737.577	C ₄₇ H ₈₅ O ₃	10.9	100	Urolithin B glucuronide
753.592	C ₄₈ H ₈₇ O ₃	10.9	100	Urolithin A glucuronide
769.607	C ₄₉ H ₈₉ O ₃	10.9	100	Urolithin B glucuronide
785.622	C ₅₀ H ₉₁ O ₃	10.9	100	Urolithin A glucuronide
801.637	C ₅₁ H ₉₃ O ₃	10.9	100	Urolithin B glucuronide
817.652	C ₅₂ H ₉₅ O ₃	10.9	100	Urolithin A glucuronide
833.667	C ₅₃ H ₉₇ O ₃	10.9	100	Urolithin B glucuronide
849.682	C ₅₄ H ₉₉ O ₃	10.9	100	Urolithin A glucuronide
865.697	C ₅₅ H ₁₀₁ O ₃	10.9	100	Urolithin B glucuronide
881.712	C ₅₆ H ₁₀₃ O ₃	10.9	100	Urolithin A glucuronide
897.727	C ₅₇ H ₁₀₅ O ₃	10.9	100	Urolithin B glucuronide
913.742	C ₅₈ H ₁₀₇ O ₃	10.9	100	Urolithin A glucuronide
929.757	C ₅₉ H ₁₀₉ O ₃	10.9	100	Urolithin B glucuronide
945.772	C ₆₀ H ₁₁₁ O ₃	10.9	100	Urolithin A glucuronide
961.787	C ₆₁ H ₁₁₃ O ₃	10.9	100	Urolithin B glucuronide
977.802	C ₆₂ H ₁₁₅ O ₃	10.9	100	Urolithin A glucuronide
993.817	C ₆₃ H ₁₁₇ O ₃	10.9	100	Urolithin B glucuronide
1009.832	C ₆₄ H ₁₁₉ O ₃	10.9	100	Urolithin A glucuronide
1025.847	C ₆₅ H ₁₂₁ O ₃	10.9	100	Urolithin B glucuronide
1041.862	C ₆₆ H ₁₂₃ O ₃	10.9	100	Urolithin A glucuronide
1057.877	C ₆₇ H ₁₂₅ O ₃	10.9	100	Urolithin B glucuronide
1073.892	C ₆₈ H ₁₂₇ O ₃	10.9	100	Urolithin A glucuronide
1089.907	C ₆₉ H ₁₂₉ O ₃	10.9	100	Urolithin B glucuronide
1105.922	C ₇₀ H ₁₃₁ O ₃	10.9	100	Urolithin A glucuronide
1121.937	C ₇₁ H ₁₃₃ O ₃	10.9	100	Urolithin B glucuronide
1137.952	C ₇₂ H ₁₃₅ O ₃	10.9	100	Urolithin A glucuronide
1153.967	C ₇₃ H ₁₃₇ O ₃	10.9	100	Urolithin B glucuronide
1169.982	C ₇₄ H ₁₃₉ O ₃	10.9	100	Urolithin A glucuronide
1185.997	C ₇₅ H ₁₄₁ O ₃	10.9	100	Urolithin B glucuronide
1201.012	C ₇₆ H ₁₄₃ O ₃	10.9	100	Urolithin A glucuronide
1217.027	C ₇₇ H ₁₄₅ O ₃	10.9	100	Urolithin B glucuronide
1233.042	C ₇₈ H ₁₄₇ O ₃	10.9	100	Urolithin A glucuronide
1249.057	C ₇₉ H ₁₄₉ O ₃	10.9	100	Urolithin B glucuronide
1265.072	C ₈₀ H ₁₅₁ O ₃	10.9	100	Urolithin A glucuronide
1281.087	C ₈₁ H ₁₅₃ O ₃	10.9	100	Urolithin B glucuronide
1297.102	C ₈₂ H ₁₅₅ O ₃	10.9	100	Urolithin A glucuronide
1313.117	C ₈₃ H ₁₅₇ O ₃	10.9	100	Urolithin B glucuronide
1329.132	C ₈₄ H ₁₅₉ O ₃	10.9	100	Urolithin A glucuronide
1345.147	C ₈₅ H ₁₆₁ O ₃	10.9	100	Urolithin B glucuronide
1361.162	C ₈₆ H ₁₆₃ O ₃	10.9	100	Urolithin A glucuronide
1377.177	C ₈₇ H ₁₆₅ O ₃	10.9	100	Urolithin B glucuronide
1393.192	C ₈₈ H ₁₆₇ O ₃	10.9	100	Urolithin A glucuronide
1409.207	C ₈₉ H ₁₆₉ O ₃	10.9	100	Urolithin B glucuronide
1425.222	C ₉₀ H ₁₇₁ O ₃	10.9	100	Urolithin A glucuronide
1441.237	C ₉₁ H ₁₇₃ O ₃	10.9	100	Urolithin B glucuronide
1457.252	C ₉₂ H ₁₇₅ O ₃	10.9	100	Urolithin A glucuronide
1473.267	C ₉₃ H ₁₇₇ O ₃	10.9	100	Urolithin B glucuronide
1489.282	C ₉₄ H ₁₇₉ O ₃	10.9	100	Urolithin A glucuronide
1505.297	C ₉₅ H ₁₈₁ O ₃	10.9	100	Urolithin B glucuronide
1521.312	C ₉₆ H ₁₈₃ O ₃	10.9	100	Urolithin A glucuronide
1537.327	C ₉₇ H ₁₈₅ O ₃	10.9	100	Urolithin B glucuronide
1553.342	C ₉₈ H ₁₈₇ O ₃	10.9	100	Urolithin A glucuronide
1569.357	C ₉₉ H ₁₈₉ O ₃	10.9	100	Urolithin B glucuronide
1585.372	C ₁₀₀ H ₁₉₁ O ₃	10.9	100	Urolithin A glucuronide

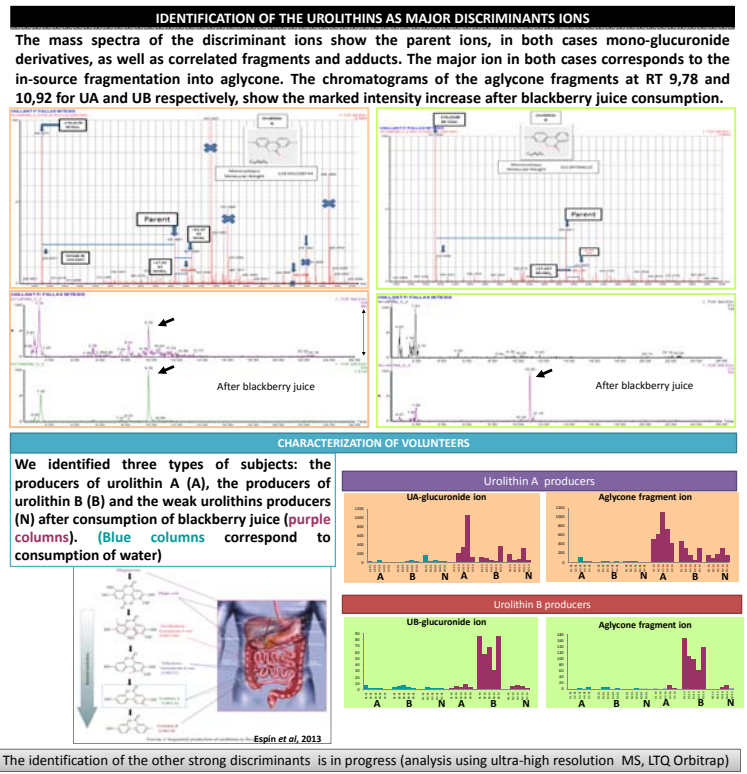
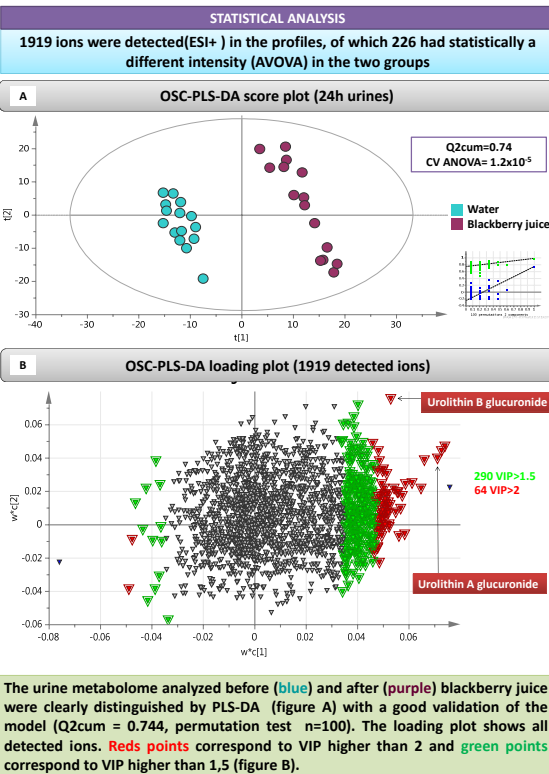
Blackberry's metabolite database creation:
Compilation of blackberry composition data

Dictionary of Food Compounds
In collaboration with the Dictionary of Food Compounds Online

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

Online databases: OEB, hmp, METLIN, PubChem

RESULTS



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.