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Title: USE OF HIGH RESOLUTION MASS SPECTROMETRY FOR IDENTIFICATION OF SPECIFIC BIOMARKERS OF COFFEE CONSUMPTION

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Abstract: As part of the ANR PhenoMeNEp project, non-targeted profiling is used to identify potential biomarkers of plant food consumption. Using 24 hour dietary recall and food frequency questionnaire data, 144 high (median 974 grams/day) and 66 low (median 305 grams/day) consumers of fruit and vegetables were selected from the French SU.VI.MAX2 cohort. Morning spot urine samples from each subject were analyzed in positive and negative ion mode by LC-MS using a QTOF mass spectrometer.

The consumption data available from the SUVI.MAX.2 cohort allows the comparison of low and high consumers of specific foods of interest. Coffee, for instance, is one of the most widely consumed beverages in the world and contains various bioactives implicated with health and the prevention of disease. The urine profiles of 20 high coffee consumers (median 290.4 ml coffee/day) and 20 non-consumers from SU.VI.MAX2 were compared. Metabolomic profiling and partial least squares discriminant analysis (PLS-DA) after orthogonal signal correction filtration (OSC) clearly distinguished low and high coffee consumption.
Among the 1112 ions found to characterize the food metabolome, 134 are statistically significant (ANOVA BH and PLS) to discriminate high and low coffee consumers. Numbers of these ions related to caffeine metabolism such as isomers of methyluric acid or methylxanthines, have been easily identified by comparison with authentic standards. Although these compounds are not really specific to coffee consumption, finding them demonstrates the relevance of the approach.
Among the most discriminating ions, three clusters were related to non-caffeine derived compounds and may be more specific to coffee consumption. Identifying unknown phytochemical metabolites is a complex task requiring the use of various analytical techniques, bioinformatics software and databases. Using LTQ-Orbitrap to access ultra high resolution and MSn experiments, in combination with prediction of MS fragmentation (Mass FrontierTM) and metabolism prediction (Meteor, Lhasa Ltd), the discriminating clusters have been tentatively identified as Atractyligenine glucuronide, Cyclo(leucyl-prolyl) and Trigonelline. Although further investigations must be carried out to qualify these compounds as specific biomarkers of coffee consumption, analytical data and knowledge of their dietary sources and metabolism make them very promising new biomarkers for nutritional epidemiology.
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