Multiple Reaction Monitoring (MRM)-Profiling to Assess Compliance With an Almond Consumption Intervention.

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Abstract:
Background: Almonds are extremely rich sources of lipids and flavonoids and their consumption is associated with several health benefits. However, there are no analytical methods available to document compliance to prescribed or self-reported chronic almond consumption. Objective: To use an analytical approach that identifies metabolic profiles associated with long-term almond consumption to ascertain compliance with prescribed consumption. Methods: A multiple reaction monitoring (MRM)-profiling strategy was designed to isolate metabolic changes in erythrocytes after 12-wk almond consumption (ClinicalTrials.gov: NCT02360787). MRM-profiling data acquisition and analysis involves performing separate discovery and screening steps to detect molecular features related to metabolic changes between experimental groups. Samples used for this research were erythrocytes recovered at baseline, after 12 weeks of almond consumption (W12-almond) and controls (W12-control). For the MRM-profiling discovery step, representative samples (pools) of erythrocytes from individuals of all groups were interrogated by precursor ion and neutral loss scan experiments based on prior knowledge of chemical functional groups present in the samples. The outputs of the discovery phase were methods used for the MRM-profiling screening phase to interrogate individual samples based on fast MRM measurements. In addition, we screened the literature for flavonoids identified in almond skins and included them for individual sample screening. Results: Out of the 254 values of m/z monitored, 5 ratios and combinations of specific ions with receiver operating characteristic curves AUC>0.89 provided sensitivity of 74.2% and specificity of 90% for blind (new samples) presented to the model. Eight out of the 31 participants (25.8%) in the W12-almond group and 3 out of the 30 (10%) participants in the W12-control group were misclassified by all 5 ratios. Ratios and combinations of specific transitions were mainly related to membrane lipids. Conclusions: The misclassifications observed as a result of ratio performance evaluation may