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Spot and Cumulative Urine Samples Are Suitable Replacements for 24-Hour Urine Collections for Objective Measures of Dietary Exposure in Adults Using Metabolite Biomarkers

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Published in:
Journal of Nutrition

DOI:
[10.1093/jn/nxz138](https://doi.org/10.1093/jn/nxz138)

Publication date:
2019

Citation for published version (APA):
Wilson, T., Garcia-Perez, I., Posma, J. M., Lloyd, A., Chambers, E. S., Tailliant, K., Zubair, H., Beckmann, M., Mathers, J. C., Holmes, E., Frost, G., & Draper, J. (2019). Spot and Cumulative Urine Samples Are Suitable Replacements for 24-Hour Urine Collections for Objective Measures of Dietary Exposure in Adults Using Metabolite Biomarkers. *Journal of Nutrition*, 149(10), 1692-1700. Article nxz138.
<https://doi.org/10.1093/jn/nxz138>

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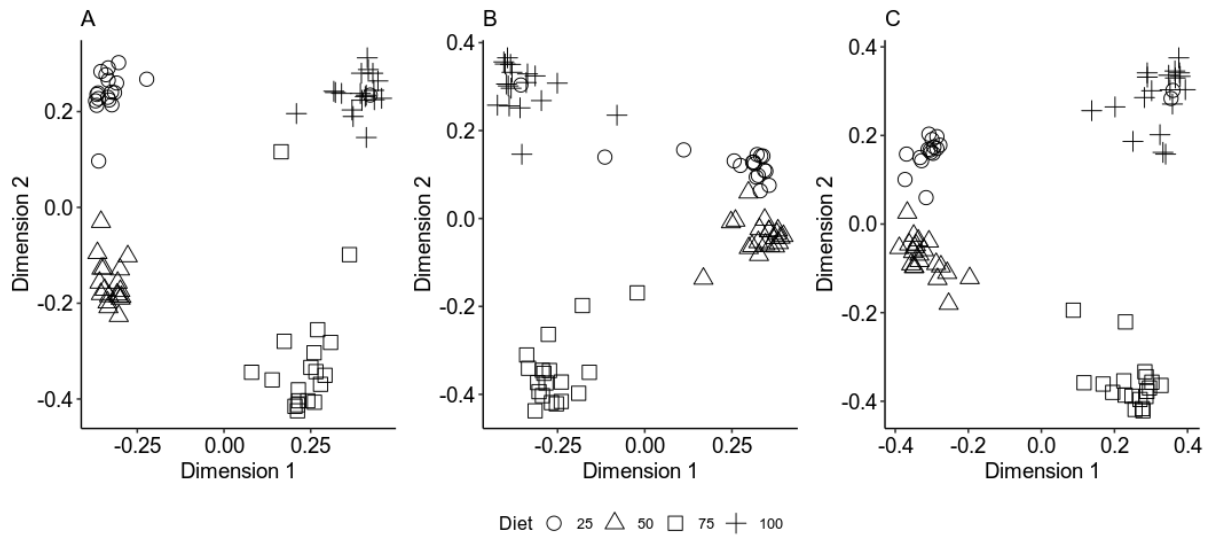
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Supplementary data

Supplemental Figure 1 Multidimensional scaling (MDS) of multinomial Random Forest classification models for diet differences in three different urine sample types

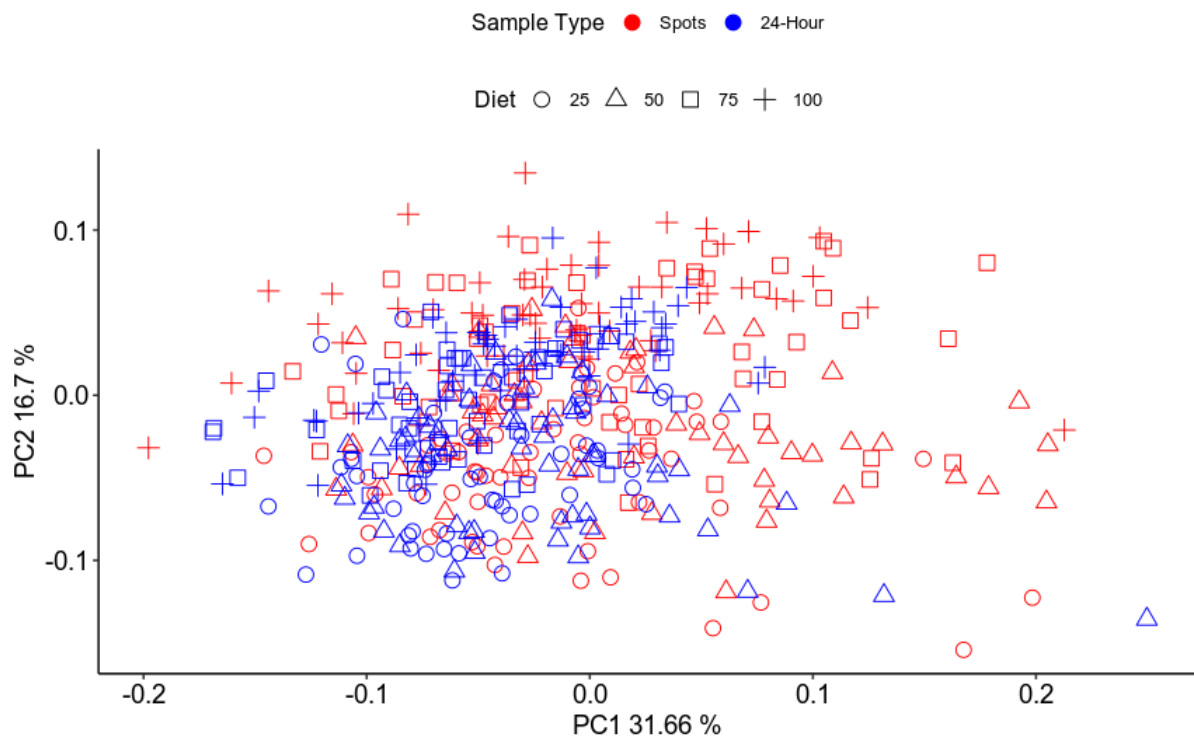


A; Post-dinner (PD) Day 2, B; Cumulative sample 3 (CS3) Day 2 and C; 24-hour Day 2.

Classification accuracies for A, B and C were 0.97, 0.96 and 0.97 respectively. Multi-class Area Under the ROC Curve (AUC) returned values of 0.98, 0.98 and 0.97 respectively.

Supplementary data

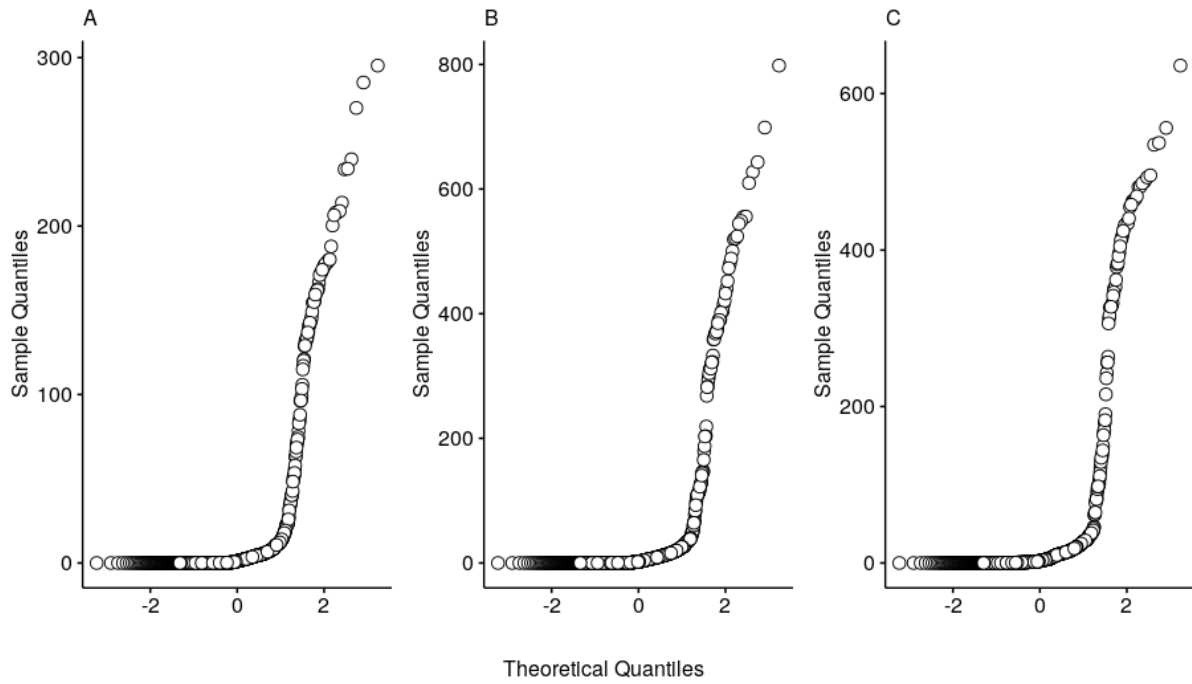
Supplemental Figure 2 Principal Component Analysis (PCA) of metabolome fingerprint data representing Post-dinner urine samples from all days of all dietary interventions with 24-hour urine sample data projected into the model



PCA was constructed using Post-dinner (PD) spot samples from all intervention days and 24-hour urine samples projected into the PCA.

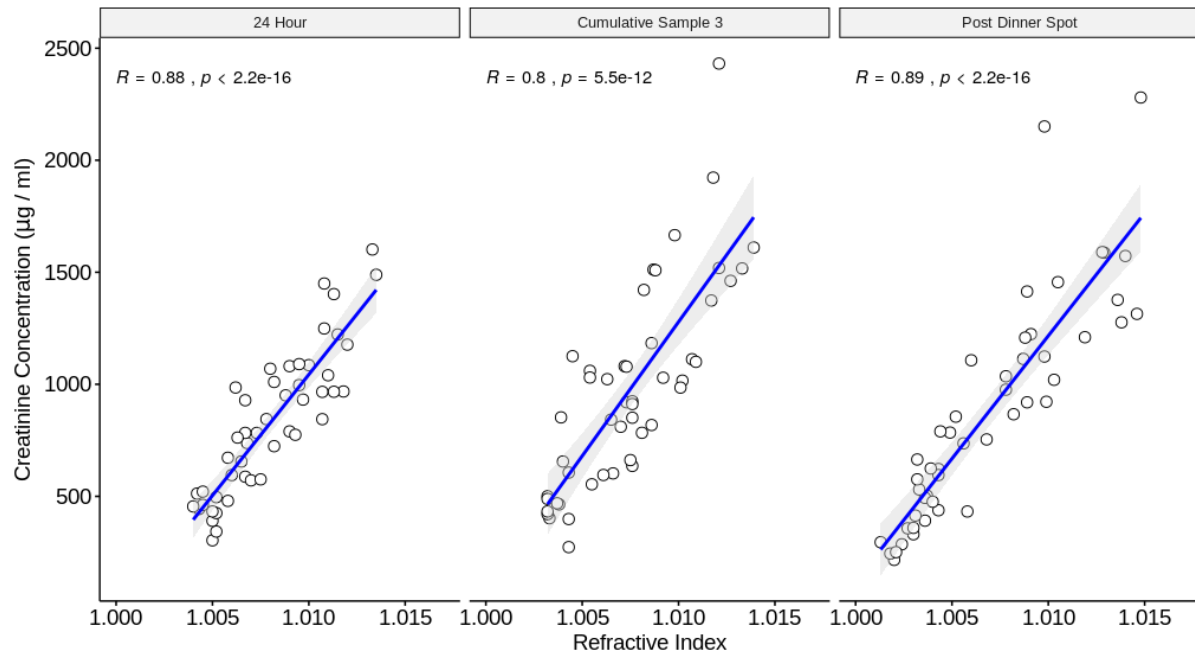
Supplementary data

Supplemental Figure 3 Quantile-Quantile (QQ) Plots of biomarker concentrations ($N = 17$) for all 19 individuals on intervention day 3 for: A; Post-dinner (PD) Spot, B; Cumulative sample 3 (CS3) and C; 24-hour urine collection.



Supplementary data

Supplemental Figure 4 Relationship between urine refractive index and creatinine concentration ($\mu\text{g/ml}$)



Scatterplot of sample refractive index and creatinine concentration ($\mu\text{g/ml}$) in three urine sample types. Pearson correlation coefficients for each sample type were as follows; 24-Hour ($\rho = 0.88$, $P < 2.2 \times 10^{-16}$), Cumulative sample 3 ($\rho = 0.80$, $P = 5.5 \times 10^{-12}$) and Post-dinner Spot ($\rho = 0.89$, $P < 2.2 \times 10^{-16}$).

Supplementary data

Supplemental Figure 5 Comparison of selected biomarker concentrations ($\mu\text{g} / \text{ml}$)

between Post Dinner spot urine and 24-Hour urine

