



Aberystwyth University

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

Wilson, Thomas; Garcia-Perez, Isabel; Posma, Joram M.; Lloyd, Amanda; Chambers, Edward S.; Tailliant, Kathleen; Zubair, Hassan; Beckmann, Manfred; Mathers, John C.; Holmes, Elaine; Frost, Gary; Draper, John

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 Measure of Dietary Exposure in Adults Using Metabolite Biomarkers. *Journal of Nutrition*, [nxz138]. <https://doi.org/10.1093/jn/nxz138>

General rights

Copyright and moral rights for the publications made accessible in the Aberystwyth Research Portal (the Institutional Repository) are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the Aberystwyth Research Portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the Aberystwyth Research Portal

Take down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

tel: +44 1970 62 2400
email: is@aber.ac.uk

Supplementary data

Supplemental Table 2 Predicted classification scores from cumulative and spot urinary models

Model sample ¹	Prediction data ²	Skilling-Mack (<i>p</i> -value) ³	Classification accuracy ⁴	Classification accuracy 95% CI ⁵
CS1-3	PB-2	3.75×10 ⁻⁰⁷	0.922	(0.914,0.930)
CS1-3	PB-3	2.38×10 ⁻⁰⁴	0.932	(0.925,0.938)
CS1-3	PL-2	1.27×10 ⁻⁰⁸	0.944	(0.938,0.949)
CS1-3	PL-3	7.60×10 ⁻⁰⁸	0.942	(0.935,0.949)
CS1-3	PD-2	2.21×10 ⁻⁰⁷	0.921	(0.913,0.928)
CS1-3	PD-3	8.28×10 ⁻¹¹	0.966	(0.961,0.970)
CS1-3	CS1-3	1.24×10 ⁻⁰⁸	1.000	(1.000,1.000)
CS1-3	CS2-3	7.85×10 ⁻¹²	0.957	(0.951,0.962)
CS1-3	CS3-3	1.49×10 ⁻⁰⁹	0.881	(0.873,0.889)
CS1-3	24H-3	9.01×10 ⁻⁰⁸	0.909	(0.902,0.916)
CS2-3	PB-2	1.03×10 ⁻⁰³	0.573	(0.559,0.588)
CS2-3	PB-3	1.00×10 ⁻⁰³	0.522	(0.508,0.535)
CS2-3	PL-2	5.85×10 ⁻⁰⁹	0.959	(0.954,0.965)
CS2-3	PL-3	2.99×10 ⁻⁰⁹	0.986	(0.983,0.989)
CS2-3	PD-2	2.42×10 ⁻⁰⁸	0.883	(0.874,0.892)
CS2-3	PD-3	6.08×10 ⁻¹¹	0.897	(0.887,0.906)
CS2-3	CS1-3	1.00×10 ⁻⁰⁷	0.755	(0.742,0.767)
CS2-3	CS2-3	1.99×10 ⁻¹¹	1.000	(1.000,1.000)
CS2-3	CS3-3	1.13×10 ⁻⁰⁹	0.759	(0.748,0.771)
CS2-3	24H-3	9.52×10 ⁻⁰⁹	0.859	(0.848,0.869)
CS3-3	PB-2	1.05×10 ⁻⁰⁴	0.701	(0.688,0.714)
CS3-3	PB-3	2.92×10 ⁻⁰³	0.736	(0.725,0.747)
CS3-3	PL-2	2.94×10 ⁻⁰⁶	0.747	(0.735,0.759)
CS3-3	PL-3	8.34×10 ⁻⁰⁸	0.748	(0.735,0.760)

CS3-3	PD-2	4.31×10^{-06}	0.988	(0.986,0.991)
CS3-3	PD-3	2.12×10^{-11}	1.000	(1.000,1.000)
CS3-3	CS1-3	3.30×10^{-06}	0.754	(0.743,0.766)
CS3-3	CS2-3	7.32×10^{-11}	0.821	(0.810,0.833)
CS3-3	CS3-3	9.69×10^{-10}	1.000	(1.000,1.000)
CS3-3	24H-3	1.40×10^{-09}	0.938	(0.931,0.946)

¹ Sample type used for model training. ² Sample type used for model prediction. ³ Skillings-Mack *p*-value are from Monte-Carlo cross validation (MCCV) of ¹H NMR data. ⁴ Classification accuracy is the resampled (*n* = 100) prediction accuracy of multinomial Random Forest classification models of FIE-HRMS data. ⁵ 95% Confidence intervals of classification accuracy values. Where Post-Breakfast (PB); Post-lunch (PL); Post-dinner (PD); Cumulative sample 1 (CS1); Cumulative sample 2 (CS2) ; Cumulative sample 3 (CS3); 24-hour urine collection (24H); 2, day 2; 3, day 3.