

## Aberystwyth University

### *Spot and Cumulative Urine Samples Are Suitable Replacements for 24-Hour Urine Collections for Objective Measures 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

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tel: +44 1970 62 2400  
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## Supplementary data

**Supplemental Table 1:** Predicted classification scores from spot and cumulative urinary models

Model sample <sup>1</sup>	Prediction data <sup>2</sup>	Skillings-Mack ( $p$ -value) <sup>3</sup>	Classification accuracy <sup>4</sup>	Classification Accuracy 95% CI <sup>5</sup>
PD-3	PB-2	$1.16 \times 10^{-02}$	0.613	(0.600,0.625)
PD-3	PB-3	$8.89 \times 10^{-04}$	0.678	(0.664,0.691)
PD-3	PL-2	$3.48 \times 10^{-06}$	0.814	(0.803,0.824)
PD-3	PL-3	$2.30 \times 10^{-10}$	0.795	(0.784,0.806)
PD-3	PD-2	$3.53 \times 10^{-06}$	0.976	(0.971,0.980)
PD-3	PD-3	$1.99 \times 10^{-11}$	1.000	(1.000,1.000)
PD-3	CS1-3	$9.43 \times 10^{-08}$	0.684	(0.671,0.697)
PD-3	CS2-3	$1.29 \times 10^{-11}$	0.969	(0.964,0.973)
PD-3	CS3-3	$2.06 \times 10^{-10}$	0.918	(0.911,0.926)
PD-3	24H-3	$4.58 \times 10^{-08}$	0.891	(0.882,0.900)
PB-3	PB-2	$2.52 \times 10^{-07}$	0.962	(0.957,0.967)
PB-3	PB-3	$1.12 \times 10^{-04}$	1.000	(1.000,1.000)
PB-3	PL-2	$6.42 \times 10^{-09}$	0.866	(0.856,0.877)
PB-3	PL-3	$5.05 \times 10^{-06}$	0.911	(0.903,0.919)
PB-3	PD-2	$2.42 \times 10^{-07}$	0.949	(0.943,0.955)
PB-3	PD-3	$8.54 \times 10^{-09}$	0.972	(0.967,0.976)
PB-3	CS1-3	$1.13 \times 10^{-06}$	0.974	(0.970,0.979)
PB-3	CS2-3	$9.84 \times 10^{-10}$	0.891	(0.883,0.899)
PB-3	CS3-3	$1.76 \times 10^{-08}$	0.895	(0.886,0.903)
PB-3	24H-3	$3.81 \times 10^{-07}$	0.910	(0.903,0.917)
PL-3	PB-2	$1.55 \times 10^{-02}$	0.730	(0.718,0.742)
PL-3	PB-3	$5.51 \times 10^{-04}$	0.810	(0.799,0.821)
PL-3	PL-2	$1.04 \times 10^{-07}$	0.962	(0.958,0.967)
PL-3	PL-3	$1.30 \times 10^{-09}$	1.000	(1.000,1.000)
PL-3	PD-2	$7.66 \times 10^{-08}$	0.911	(0.903,0.919)

PL-3	PD-3	$5.05 \times 10^{-11}$	0.872	(0.863,0.881)
PL-3	CS1-3	$2.37 \times 10^{-07}$	0.844	(0.834,0.854)
PL-3	CS2-3	$3.27 \times 10^{-11}$	0.975	(0.971,0.979)
PL-3	CS3-3	$2.95 \times 10^{-09}$	0.861	(0.852,0.87)
PL-3	24H-3	$1.99 \times 10^{-06}$	0.896	(0.887,0.904)

<sup>1</sup>Sample type used for model training. <sup>2</sup>Sample type used for model prediction. <sup>3</sup> Skillings-Mack *p*-value are from Monte-Carlo cross validation (MCCV) of <sup>1</sup>H NMR data. <sup>4</sup> Classification accuracy is the resampled ( $n = 100$ ) prediction accuracy of multinomial Random Forest classification models of FIE-HRMS data. <sup>5</sup> 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.