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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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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.