Development of a pipeline for exploratory metabolic profiling of infant urine

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Supporting Information Legends.

Figure S1. Schematic of urine extraction via centrifugation apparatus to extract urine from cotton wool

Figure S2. Urine dilution series and 1D ^{1}H NMR experimental design

Figure S3. Principal Components Analysis (PCA) scores scatter plot showing cotton ball and diaper contamination urine profiles analyzed by 1D ^{1}H NMR spectroscopy. Key: star = blank urine; circles= urine from cotton wool balls not subject to freeze thaw cycle; squares = urine from cotton wool balls subject to freeze thaw cycle; triangles = urine from diapers and cotton wool balls

Figure S4. Orthogonal Projections to Latent Structures Discriminant Analysis (O-PLS-DA) loadings coefficients plot showing discriminatory metabolites separating between a cotton wool ball that was squeezed (negative direction) vs centrifuged (positive direction) – contaminants 1: Isobutanol (δ0.88, -CH3), 2: Tert-butanol (δ1.25, -CH3) 3: Acetone (δ2.23, -CH3).

Figure S1

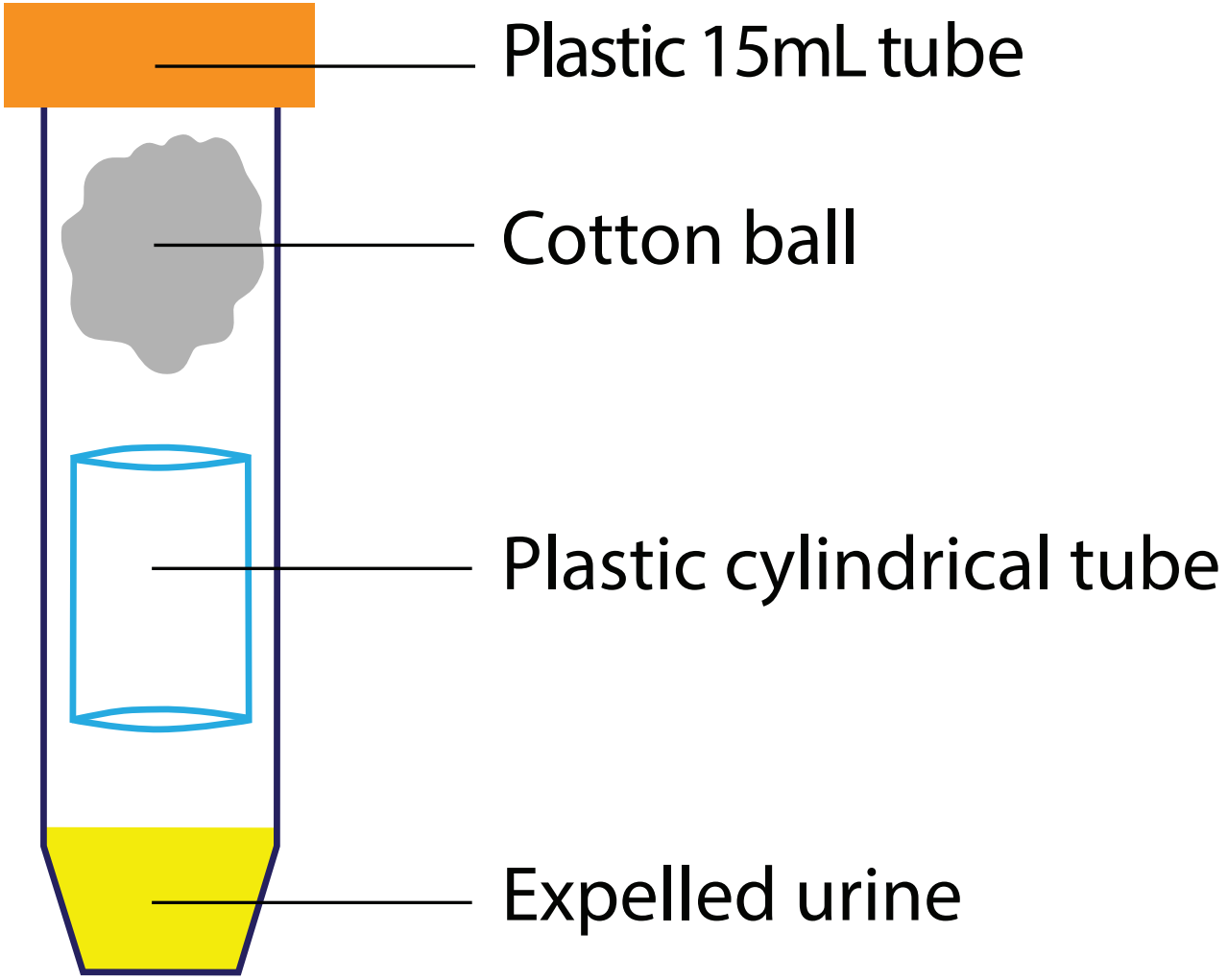
Plastic 15mL tube
Cotton ball
Plastic cylindrical tube
Expelled urine

Figure S2

Urine volume	Volume of water (ml)	Volume of phosphate buffer (ml)	Number of acquisitions performed
Volume 1: 540ml	0	60	32
Voume 2: 270ml	270	60	32
			128
Voume 3: 135ml	405	60	32
			512
Voume 4: 68ml	472	60	32
			2048

Figure S3

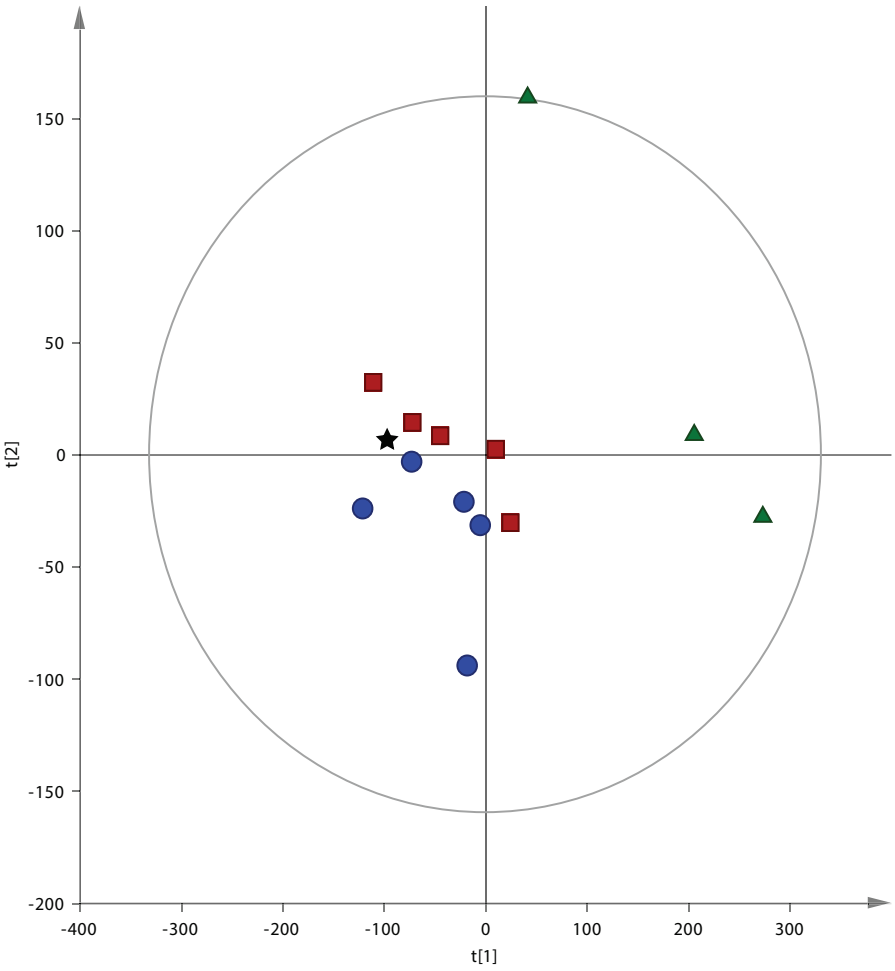

Figure S4