Additional Methods

Chemical Analysis

Samples were allowed to equilibrate to room temperature prior to transferring 0.975 ml of the sample to a 1.5 ml screw cap, amber GC vial. 25 µL of the Internal Standard (containing Caffeine-D9, Codeine-D6, Carbamazepine-D10, Acetaminophen-D4, Cotinine-D3 and Acesulfame-D4) was then added to the GC vial and the vial was shaken for 5 s. Two blanks of HPLC-grade water are treated the same way and included in each set to monitor any contamination. A Waters Xevo TQ-S system equipped with a Kinetex Biphenyl analytical column (3x100 mm i.d., 2.6 µm particle size) was used to separate the compounds at a column temperature of 40°C and flow rate of 400 µl/min. The mobile phase solvents were water (A) and methanol (B), each containing 0.1% formic acid and 10 mM Ammonium Acetate. The compounds were separated by the following gradient: 50% A & 50% B at time = 0 minute and 5% A & 95% B at time = 1 minute (& held for duration of the 6 minute run). The column was allowed to equilibrate for 5 min between each injection. The injection volume was 50 µL and all compounds were analysed using a Waters Xevo TQ-S UHPLC-MS/MS with an Electrospray Ionization (ESI) source utilizing polarity switching. The optimized ESI-MS/MS conditions were as follows: desolvation gas = 1000 L/hr, collision gas = 0.18 ml/min, cone gas = 150 L/hr, capillary voltage = 0.70kv, source temperature = 150°C and desolvation temperature = 600°C. The dwell time per ion-pair is optimized to obtain at least 12 points/peak.

An 8-point standard curve spanning 4 orders of magnitude was used to quantify using a linear relationship with R^2>0.99. The calibration curve and analyte chromatograms were checked for calibration linearity of R^2>0.985, symmetrical peak shapes, well-resolved and

properly-integrated peaks, and consistency of the internal standard peaks. Samples were not blank-corrected. A compound was reported as positively identified when the compound was observed at the known retention time (± 0.02 min), and the ratio of the qualifying ion to quantifying ion (cps) was within the acceptable range. The requirement for each qualifier ion was that its integrated peak area falls within a range of specified ratios with respect to the peak area of the quantifier ion. As long as the retention time and ratio of areas falls within their respective ranges, the acceptance criteria for confirmation were met.

Table S1. Selected-ion monitoring (SIM) program and retention times for analysis of target compounds

Compound	ESI Mode	Quantitation & Qualifier Ion Pairs (m/z)	Ratio Qual/Quant Peak Area (± Limit)	V_f (v)	Retention Time (min)
Caffeine D9	+	204 - 144	Internal standard		
Cotinine D3	+	180 - 80	Internal standard		
Codeine D6	+	306.2 – 165.1	Internal standard		
Carbamazepine D10	+	237.1 – 194.1	Internal standard		
Acetaminophen D4	+	156 - 114	Internal standard		
Acesulfame D4	-		Internal standard		
Caffeine	+	195.2 – 110.2 195.2 – 138.1	100% (± 20%)	33 30	2.71
Cotinine	+	177.2 – 80.1 177.2 - 98	23% (± 25%)	34 33	2.15
Codeine	+	300.3 – 165 300.3 - 152	80% (± 20%)	45 60	1.61
Carbamazepine	+	247.1 – 204.1	N/A	38	4.73
Acetaminophen	+	152.1 – 110.0 152.1 – 65.1	100% (± 20%)	25 30	1.37
Acesulfame	-	162.1 – 82 162.1 - 78	15% (± 30%)	16 20	1.2
Sucralose	-	395.1 – 359.1	N/A	12	1.51