Supporting Information for:

Strategies for nonpolar aerosol collection and heavy metals analysis of inhaled cannabis products

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Supporting Information for Publication

Table S1: *Concentration of 10 metals measured before and after spiking cannabis concentrate and flower in µg/g. Each value is the average of three samples and uncertainty is the standard deviation.*

Metal	Isotope	Cannabis concentrate		Cannabis Flower		10% Terpene Distillate	
		Blank/stock Concentrate	***Spiked Concentrate***	***Blank/stock Flower***	***Spiked Flower***	***Unpiked Distillate***	***Spiked Distillate***
As	75	<LOD*	7.33 ± 0.67	0.0617 ± 0.0145	8.87 ± 0.79	<LOD*	10.0 ± 0.6
Cd	111	<LOD*	7.57 ± 0.93	0.0391 ± 0.0060	8.50 ± 1.35	<LOD*	8.97 ± 0.54
Co	59	<LOD*	7.99 ± 0.39	0.102 ± 0.013	9.45 ± 1.02	<LOD*	11.6 ± 0.4
Cr	52	0.153 ± 0.018	8.02 ± 0.29	0.162 ± 0.054	9.94 ± 1.17	<LOD*	9.48 ± 0.40
Cu	63	0.318 ± 0.488	8.35 ± 0.42	26.7 ± 11.0	25.9 ± 3.17	<LOD*	9.27 ± 0.50
Hg	202	0.254 ± 0.146	3.44 ± 0.68	<LOD*	8.28 ± 1.59	<LOD*	2.61 ± 0.07
Mn	55	0.529 ± 0.059	8.42 ± 0.23	149 ± 10	218 ± 12	<LOD*	9.85 ± 0.47
Ni	58	0.0885 ± 0.0134	8.01 ± 0.48	1.84 ± 0.29	12.3 ± 1.3	0.0447 ± 0.0298	11.5 ± 0.3
Pb	207	<LOD*	8.62 ± 0.51	0.160 ± 0.034	10.3 ± 3.4	<LOD*	10.3 ± 0.3
Sn	118	<LOD*	9.85 ± 1.71	0.445 ± 0.048	13.6 ± 1.7	<LOD*	7.73 ± 2.63

**LOD data can be found in Table 3 of the main publication text.*

Table S2. *Cannabinoid content of model system cannabis concentrate in weight percent as determined by reverse-phase UHPLC. Data points were taken in triplicate and averaged, the uncertainty is the standard deviation. CBD = cannabidiol, CBN = cannabinol, THC= tetrahydrocannabinol, THCA=tetrahydrocannabinolic acid*

	CBD	**CBN**	**Δ9-THC**	**Δ8-THC**	**THCA**	**CBG**	**CBC**
Blank concentrate (no terpenes)	13.52 ± 0.12	2.2 ± 0.02	21.14 ± 0.23	0 ± 0	28.2 ± 0.31	<LOD	<LOD
Spiked concentrate (no terpenes)	2.55 ± 0.03	2.16 ± 0.01	24.01 ± 0.18	5.26 ± 0.08	21.2 ± 0.25	<LOD	<LOD
Blank distillate (10% terpenes)	<LOD	0.32 ± 0.04	75.1 ± 1.4	<LOD	<LOD	0.57 ± 0.02	0.26 ± 0.03
Spiked disillate(10% terpenes)	<LOD	0.51 ± 0.02	68.58 ± 1.59	<LOD	<LOD	0.33 ± 0.01	5.41 ± 0.13

Table S3: *Concentration of terpenes in spiked concentrate material (mg/g) as determined by GC-FID. Samples were analyzed in triplicate and averaged, the uncertainty is the standard deviation.*

Terpene	**Average Concentration (no terpenes added) (mg/g)**	**Average Concentration (10% terpenes) (mg/g)**
α-Pinene	0.729 ± 0.039	11.3 ± 2.8
Camphene	<LOD	0.269 ± 0.209
β-Myrcene	0.445 ± 0.136	9.35 ± 2.36
β-Pinene	<LOD*	1.02 ± 0.52
3-Carene	<LOD*	0.567 ± 0.268
α-Terpinene	<LOD*	<LOD*
Limonene	1.70 ± 0.097	8.03 ± 1.95
p-Cymene	<LOD*	<LOD*
Ocimene 1	<LOD*	<LOD*
Eucalyptol	<LOD*	<LOD*
γ-Terpinene	<LOD*	<LOD*
Tepinolene	<LOD*	<LOD*

Linalool	0.605 ± 0.027	0.147 ± 0.150
Isopulegol	<LOD*	<LOD*
Gaeraniol	<LOD*	0.044 ± 0.063
β-Caryophyllene	2.09 ± 0.645	5.18 ± 1.64
α-Humulene	0.110 ± 0.150	2.62 ± 0.90
cis-Nerolidol	<LOD	0.159 ± 0.186
trans-Nerolidol	<LOD*	<LOD*
Guaiol	<LOD*	<LOD*
Caryophyllene Oxide	1.81 ± 0.11	<LOD*
α -Bisabolol	4.64 ± 0.37	1.05 ± 0.52

LOD for Terpene assay is 0.05 mg/g

Table S4: *Concentration of various residual solvents in spiked concentrate material in µg/g as determined by GC-FID headspace injection. Data points were taken in triplicate and averaged, the uncertainty is the standard deviation.*

Solvent Name	**Concentration (no terpenes) (*µg/g*)**	**Concentration (10% terpenes) (*µg/g*)**	**LOD (µg/g)**	**LOQ (µg/g)**
Propane	<LOD	<LOD	7.40	24.66
Isobutane	<LOD	<LOD	2.16	7.20
n-Butane	<LOD	<LOD	1.87	6.24
Methanol	<LOD	<LOD	4.96	16.51
n-Pentane	<LOD	<LOD	1.29	4.31
Ethanol	<LOD	<LOD	3.81	12.69
Ethyl Ether	<LOD	<LOD	4.20	13.98
Acetone	38.2 ± 9.4	<LOD	4.66	15.53
2-Propanol	19.3 ± 2.0	1120 ± 50	4.73	15.74
Acetonitrile	<LOD	<LOD	6.47	21.53
Dichloromethane	<LOD	<LOD	12.72	42.34
n-Hexane	<LOD	<LOD	1.44	4.78
Ethyl Acetate	<LOD	<LOD	7.83	26.07
Cyclohexane	<LOD	<LOD	7.46	24.85
Benzene	<LOD	<LOD	0.22	0.74
n-Heptane	<LOD	<LOD	10.36	34.50
Toluene	<LOD	<LOD	16.64	55.41
Ethyl Benzene	<LOD	<LOD	5.88	19.59
m, p-Xylene	<LOD	<LOD	14.21	47.31
o-Xylene	<LOD	<LOD	10.20	33.98

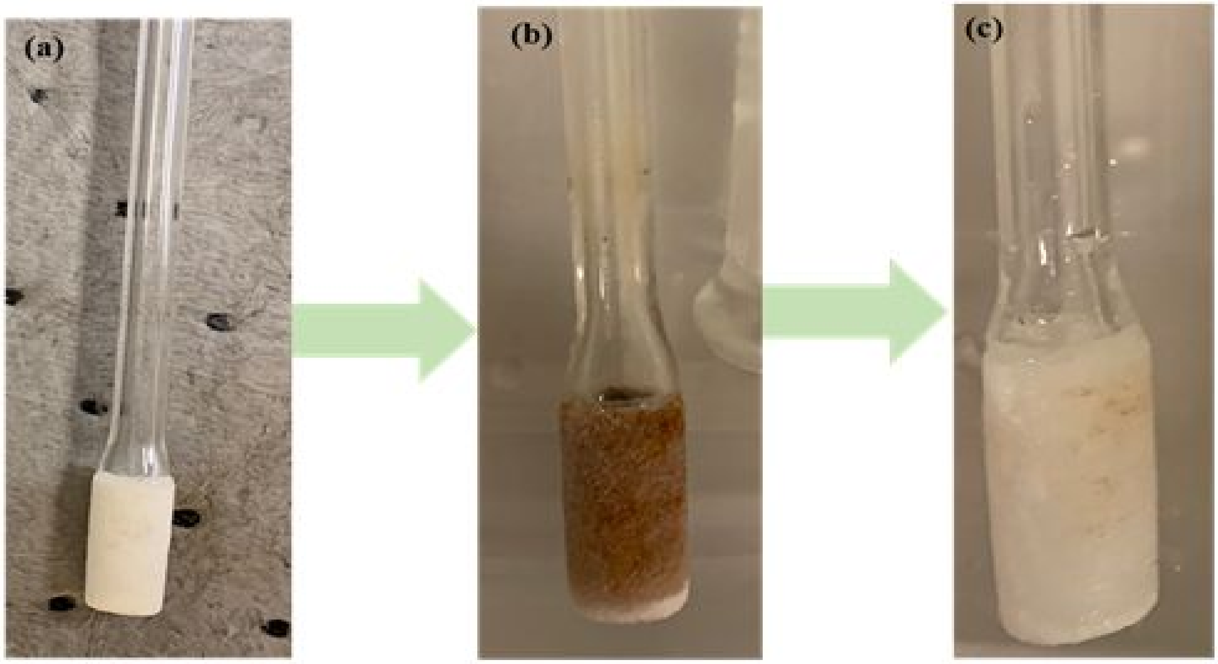

Figure S1. *Images of fritted glass impinger insert that diffuses the incoming aerosol mixtures into the liquid solvents. a) Clean insert before vaping session (a), clogged frits after vaping cannabis concentrate in an aqueous impinger, showing oil droplets or aerosols condensing on inside of fritted materials (b), after vaping cannabis concentrate in an organic solvent showing the oil droplets do not remain in the frits(c). The organic solutions in the impinger vessels had a yellow-brown color indicating the oil dissolved into the solvent and was not trapped in frits. Open-ended impinger inserts were investigated, but did not allow for small bubble formation and resulted in loss of vapor seen visibly traveling through the system into the smoke box.*

Investigation of filter paper usage during aerosol collection Initially, it was thought that a filter paper placed before the impingers could be used to increase metals capture. Moderate increases in recovery were demonstrated for some metals using Whatman Ashless 41 filter papers (CAT no. 1441-047) (see Figure S2). However, it was shown across many trials that even blank filter paper controls could provide substantial background signals. Several other types of filters were also tested and all of them provided inconsistent and large background signals (Figure S3). Another significant reason for the discontinued usage of filters in these trials is that they would frequently become saturated with oil after only a small number of puffs and restrict airflow, causing inconsistent volumes to be puffed (as measured with a flowmeter—data not shown).

The final reason that filter papers were not included is that their full digestion and separate analysis created excessive time and cost to the method for marginal increases in metal recovery.

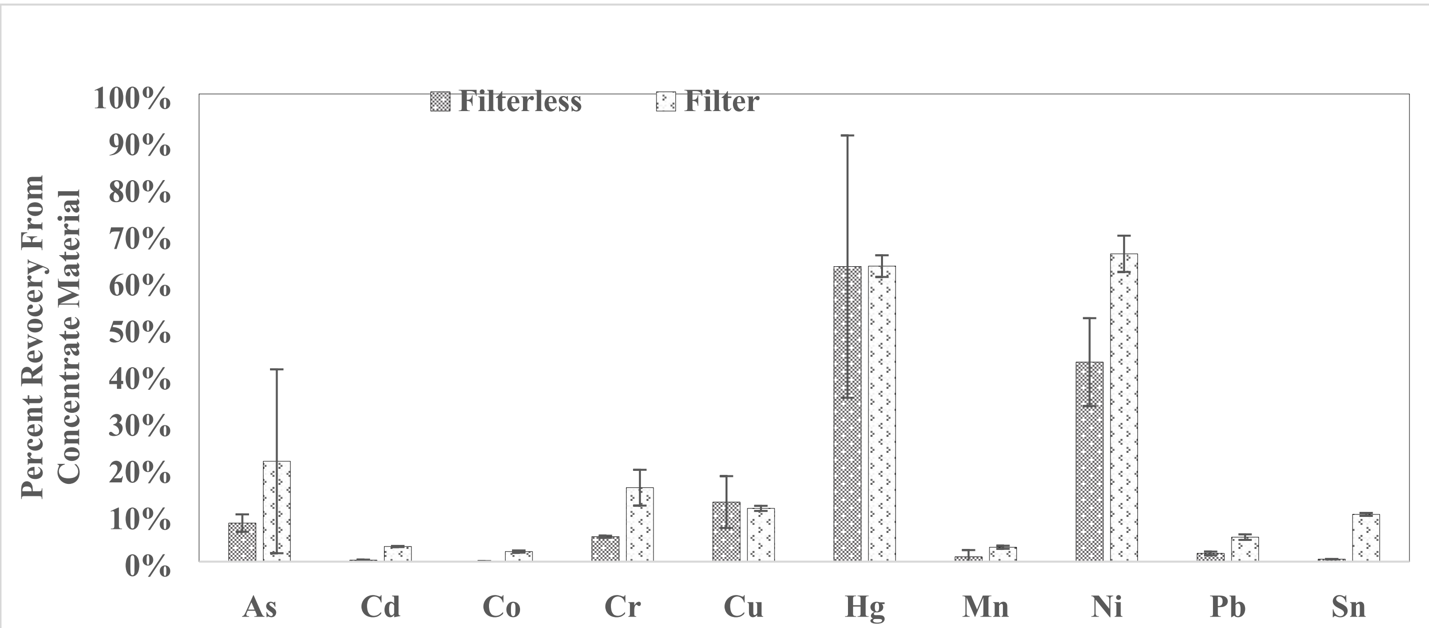

Figure S2. *Percent recovery of metals with and without filter paper in the aerosol collection stream from spiked concentrate material. Whatman Ashless 41 filter papers (CAT no. 1441-047) were used. Data is presented as % of original spiked amount for each metal, error bars are standard deviation of three trials. Notably, this data was taken before solvent trials were performed, which means that these samples were taken from preliminary aqueous impinger solvent data (2AA collection method).*

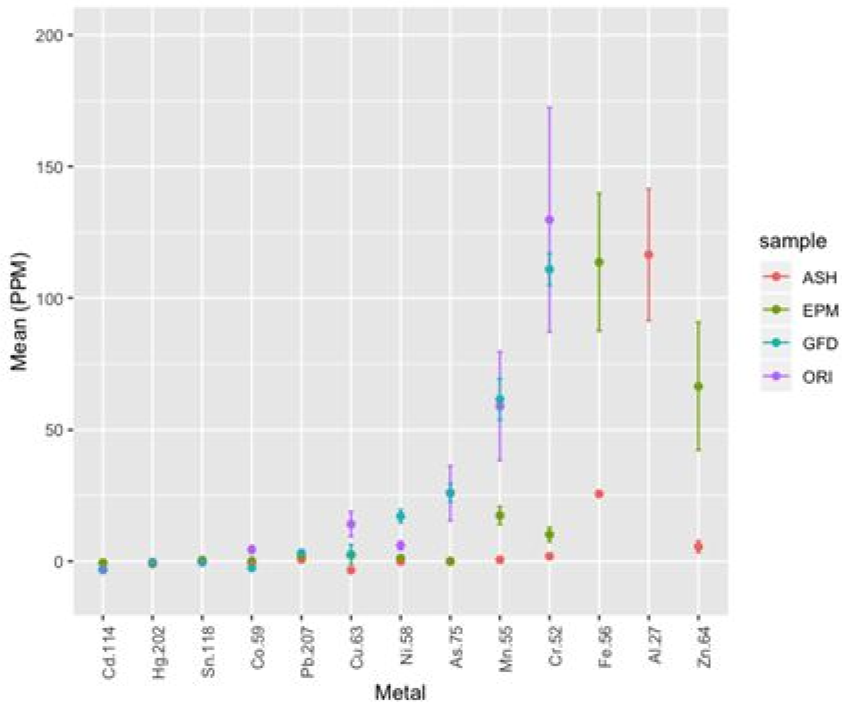

Figure S3. *Concentrations of metals found in various types of unused filter paper. ORI=the original filter paper that came with smoke machine [Brand undisclosed]. GFD= glass microfiber filter designed for fast flow rates and membrane protection [Whatman 1823-047], EPM=air sampling filter made from 100% borosilicate designed for analytical sampling with minimal interference [Whatman 1882-047], ASH=Ashless filter paper designed for residue free burning [Whatman 1441-047]. Fe, Al and Zn are off the scale of this graph for GFD and ORI papers.*