SUPPORTING INFORMATION:

Evaluation of e-vapor nicotine and nicotyrine concentrations under various e-liquid compositions, device settings, and vaping topographies

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I. Vaping topography measurements

The demographics of the study participants are summarized in Table S1.

Table S1. Summary of the study participants

Number of study participants	23
Age	25 ± 10 (18-52) years
Gender	21 men and 2 women
Ethnicity	16 White; 1 Black; 3 Asian; 6 others
Duration of e-cigarette use	1.4 ± 0.9 (0.4-4.0) years

Table S2 shows the mean, the standard deviation, and the range of e-cigarette vaping topography, device power output, and nicotine contents of the 23 study participants in our study. E-cigarette device power output ranged from 5 watts to 59.7 watts, with an average power output of 13.7 watts. The average nicotine content in e-liquids was 11.9 ± 10.0 mg/mL, with a maximum nicotine level of 36 mg/ml. Most subjects used vegetable glycerin (VG) based e-liquids (14 participants), followed by PG:VG mixed e-liquids (7 participants), and PG-based e-liquids (2 participants).

Table S2. Vaping topographies, e-cigarette device power settings, and nicotine contents in e-liquids across the 23 study participants

Parameters	Mean	Standard Deviation	Percentiles						
			Min	10	25	50	75	90	Max
Puff volume (mL)	100.17	55.57	9.99	38.39	63.58	90.04	135.62	160.46	251.13
Puff duration (sec)	3.69	1.16	1.26	2.08	3.24	3.85	4.24	5.06	5.77
Puff interval (sec)	24.30	17.30	8.01	11.90	13.86	18.67	26.35	67.91	69.39
Power (W)	13.70	15.14	5.00	5.48	6.26	7.61	12.96	27.38	59.67
Nicotine (mg/mL)	11.92	10.04	0.00	3.00	3.00	12.00	19.50	24.00	36.00

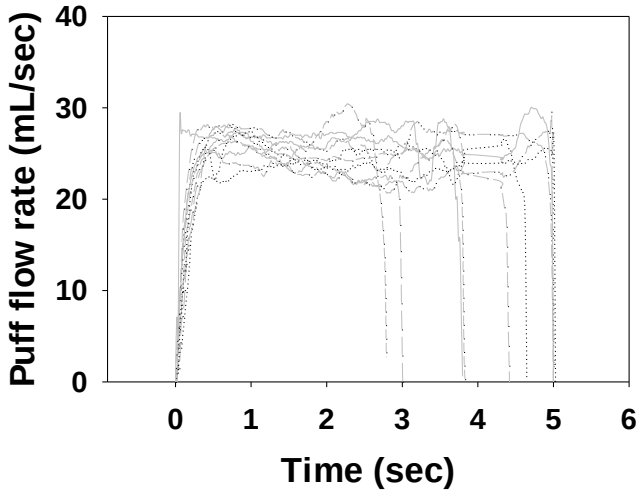

Figure S1. Observed e-cigarette puff patterns using the Cress pocket device for the study participants

II. The experimental settings for e-cigarette particle generation

E-cigarette particles were generated under the following conditions specified in Table S3.

Table S3. The experimental settings for e-cigarette particle generation

Experiments	Factors	Settings	Other Settings
E-liquid bulk material	Base material	PG, VG, PG&VG (v:v = 1:1)	6.4 W, 2 mm air hole, 90 mL puff volume, 3.8 sec puff duration
	Nicotine (mg/mL)	0, 3, 12, 24, 36	
Device setting	Device power (watt)	6.4, 14.7, 31.3	2 mm air hole, 90 mL puff volume, 3.8 sec puff duration, and 12 mg/ml nicotine in VG
Vaping topography	Puff volume (mL)	35, 90, 170	6.4 W, 2 mm air hole and 12 mg/ml nicotine in VG
	Puff duration (sec)	2, 3.8	

***Strawberry (Ripe), dragonfruit, menthol, cinnamon, bubblegum, bavarian cream, sweet cream, and graham cracker**
****0.1% and 1% for the cinnamon flavor**

III. The calibration curves for nicotine and nicotyrine

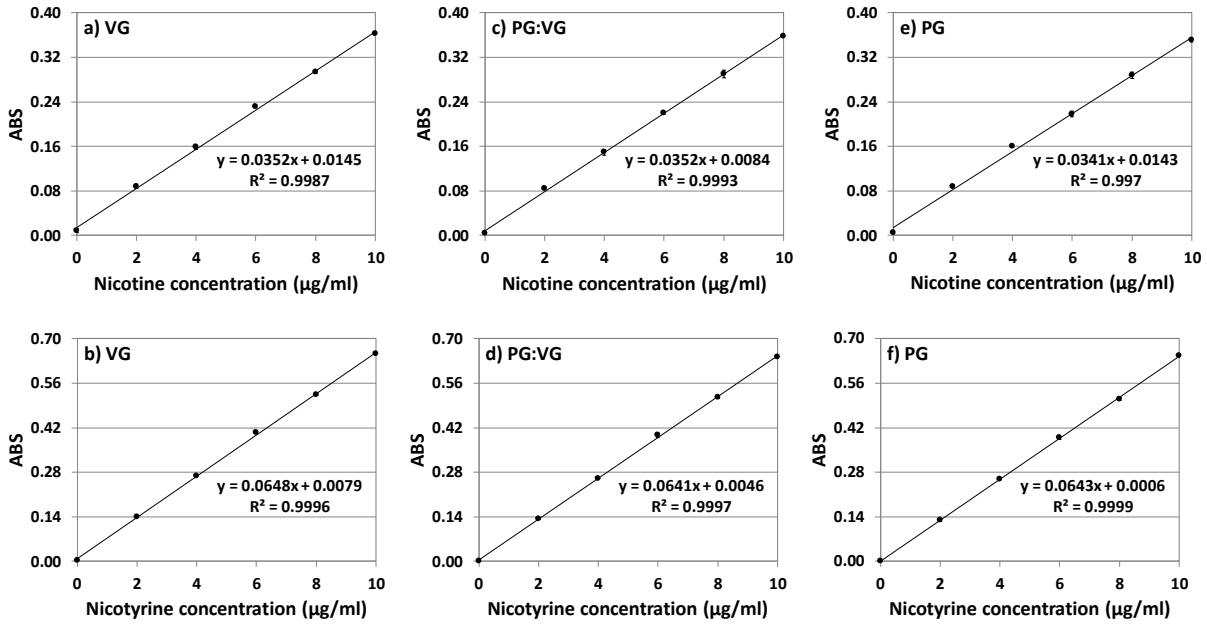

Figure S2. Nicotine and nicotyrine calibration curves prepared using 100% VG (a, b), 50% of PG and 50% of VG mixture (c, d), and 100% PG based e-liquid (e,f)

IV. Nicotine and nicotyrine analysis using GC/MS/MS method

In order to measure nicotine and nicotyrine concentrations of e-vapor using GC/MS/MS, 20 puffs of e-vapor were generated using VG based e-liquid containing 12 mg/ml nicotine under the two different power output conditions (6.4W and 31.3W). Vaping topography was 90 ml puff volume , 3.8-sec puff duration, and 24-sec puff interval. Generated e-vapor was collected on the Teflon filter, and then the sample filter was spiked using 2 µl quinoline to have the final concentration of 545 µg/ml. Extracted e-vapor with 4 ml of methanol (HPLC grade, ≥99.9%, Sigma, St. Louis, MO, USA) was analyzed using multiple reaction monitoring (MRM) mode using the parameters tabulated in Table S4.

Table S4. GC/MS/MS parameters

Compound	Retention time (min)	Parent (m/z)	Daughter (m/z)	Collision energy (V)
Quinoline	8.59	129	77	35
		129	103	25
Nicotine	12.36	162	84	11
Nicotyrine	17.71	158	130	28

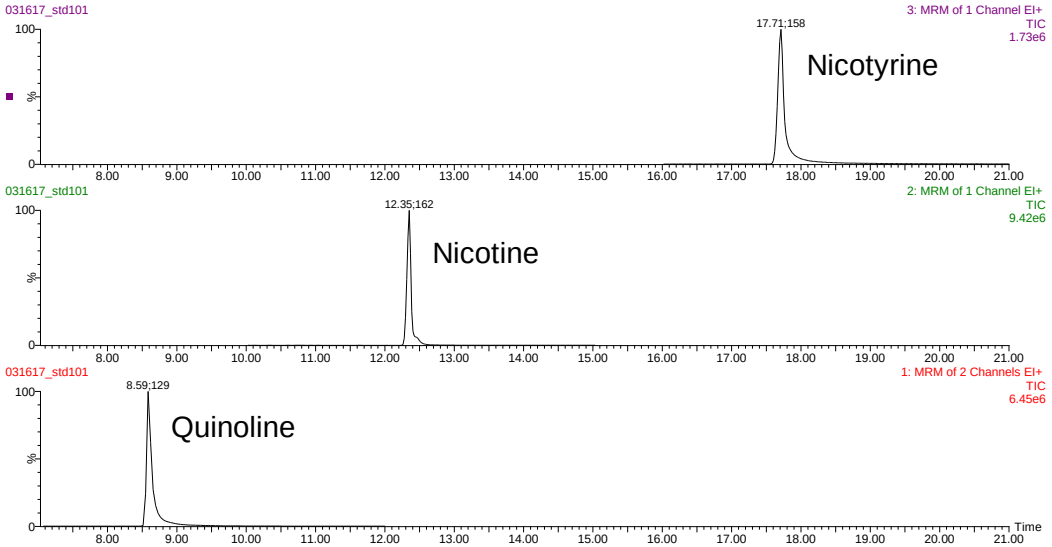

Figure S3. Chromatographic profiles of quinoline, nicotine, and nicotyrine

All GC/MS/MS analysis was performed using the Waters Micromass Quattro micro GC (Waters Corporation, Milford, MA, USA) connected with the Agilent 6890N GC oven (Agilent Technologies, Santa Clara, CA, USA). A DB-5ms column (30 m length, 0.25 mm ID, 0.25 µm thickness, Agilent Technologies, Santa Clara, CA, USA) was installed in splitless mode. The GC oven temperature ramp 80 °C for 2 min, 4 °C /min to 125 °C, hold 5 min, 40 °C/min to 240 °C, hold 5min. Constant flow rate was used with a He flow of 2 ml/min. Figure S2 shows chromatographic profiles of quinoline, nicotine, and nicotyrine.

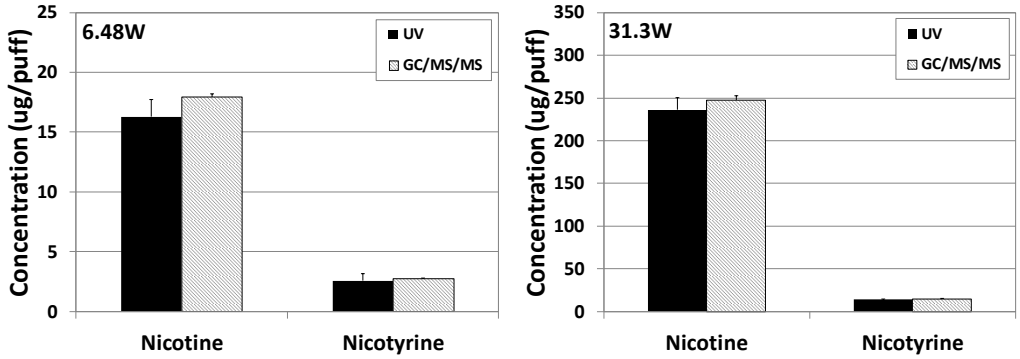

Figure S4. Nicotine and nicotyrine concentration measured using UV and GC/MS/MS method (N = 3, and error bars are standard deviations of the 5 independent measurements)

Figure S4 shows nicotine and nicotyrine concentration measured using UV and GC/MS/MS method. Average extraction efficiency was 99.4±0.7%. No significant difference was observed between these two methods, with the average difference less than 10%.

V. Calibration factors for the sampling artifacts

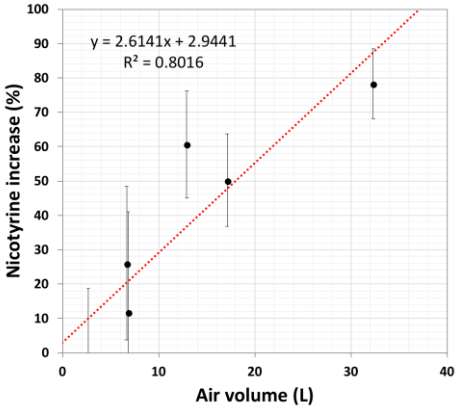

Figure S5. Linear regression for the introduced air volume (L) into the sample filter and nicotyrine increment (%). Point and error bar indicates mean and standard deviation (n=5)

Table S5. Calibration factors for the air introduced into the sample filters

Puff duration	Puff volume		
	35 ml	90 ml	170 ml
2 sec	0.938	0.890	0.828
3.8 sec	0.910	0.828	0.731

Calibration factors for the sampling artifacts were derived using the relationship between the air introduced into the sample filter (L) and increased nicotyrine by percentage (Figure S5). Estimated calibration factors were tabulated in Table S5. Calibration factors for the e-liquid samples with different nicotine concentrations were 0.423, 0.828, 0.945, and 0.962 for 3, 12, 24, and 36 mg/ml, respectively.

VI. Nicotine, nicotyrine and e-vapor mass under different experimental conditions

Table S6. Nicotine, nicotyrine, nicotyrine/nicotine ratio, and e-vapor mass of e-cigarette vapor generated from e-liquid with different base material and nicotine contents

Base Material	Component	Nicotine Contents			
		3 mg/mL	12 mg/mL	24 mg/mL	36 mg/mL
VG	Nicotine (μg/puff)	3.87±0.51	15.74±2.90	30.45±5.03	45.15±2.67
	Nicotyrine (μg/puff)	0.19±0.06	1.98±0.38	2.55±0.35	2.59±0.43
	Nicotyrine/Nicotine	0.050±0.019	0.126±0.041	0.084±0.019	0.057±0.019
	E-vapor mass (mg/puff)	1.59±0.21	1.53±0.20	1.25±0.05	1.34±0.27
	Nicotine (mg/ml)	1.93±0.36	8.19±1.86	19.3±3.27	26.8±5.68
PG:VG = 1:1	Nicotine (μg/puff)	4.54±1.00	17.33±2.23	29.5±2.08	43.1±4.71
	Nicotyrine (μg/puff)	0.23±0.05	1.67±0.28	2.53±0.19	2.62±0.25
	Nicotyrine/Nicotine	0.050±0.096	0.096±0.046	0.086±0.023	0.061±0.011
	E-vapor mass (mg/puff)	1.33±0.27	1.38±0.42	1.41±0.24	1.31±0.09
	Nicotine (mg/ml)	2.97±0.89	10.9±3.61	18.3±3.38	28.6±3.69
PG	Nicotine (μg/puff)	0.37±0.03	2.13±0.15	3.80±0.36	7.55±0.38
	Nicotyrine (μg/puff)	0.01±0.00	0.24±0.05	0.35±0.11	0.72±0.21
	Nicotyrine/Nicotine	0.025±0.007	0.114±0.035	0.091±0.035	0.096±0.041
	E-vapor mass (mg/puff)	0.18±0.03	0.16±0.02	0.16±0.02	0.20±0.05
	Nicotine (mg/ml)	1.99±0.33	12.7±2.16	23.1±3.88	35.5±8.19

Table S7. Nicotine, nicotyrine, nicotyrine/nicotine ratio, and e-vapor mass of e-cigarette vapor generated under different E-cigarette device power outputs

Component	Device Power		
	6.4 W	14.7 W	31.3 W
Nicotine (μg/puff)	16.3±1.44	137.1±6.72	236.3±13.97
Nicotyrine (μg/puff)	2.11±0.51	12.7±0.34	11.6±0.35
Nicotyrine/Nicotine	0.129±0.043	0.092±0.030	0.049±0.005
E-vapor mass (mg/puff)	1.47±0.22	8.90±2.06	21.3±1.19
Nicotine (mg/ml)	8.82±1.54	8.64±2.10	8.70±0.71

Table S8. Nicotine, nicotyrine, nicotyrine/nicotine ratio, and e-vapor mass of e-cigarette vapor under different vaping topographies

Puff duration	Component	Puff volume		
		35 ml	90 ml	170 ml
2 sec	Nicotine (μg/puff)	3.29±0.31	3.05±0.26	3.53±0.39
	Nicotyrine (μg/puff)	0.23±0.02	0.24±0.01	0.23±0.01
	Nicotyrine/Nicotine	0.069±0.014	0.078±0.015	0.064±0.033
	E-vapor mass (mg/puff)	0.31±0.03	0.28±0.03	0.33±0.12
	Nicotine (mg/ml)	8.48±1.18	8.68±1.28	8.43±3.15
3.8 sec	Nicotine (μg/puff)	10.8±2.03	16.0±0.74	24.4±1.91
	Nicotyrine (μg/puff)	2.19±0.25	2.28±0.38	2.65±0.25
	Nicotyrine/Nicotine	0.202±0.053	0.142±0.044	0.109±0.017
	E-vapor mass (mg/puff)	0.94±0.09	1.43±0.26	2.25±0.15
	Nicotine (mg/ml)	9.13±1.94	8.91±1.67	8.58±0.88