

SUPPORTING INFORMATION:

Hydroxyl Radicals in E-cigarette Vapor and E-vapor Oxidative Potentials under Different Vaping Patterns

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TABLE OF CONTENTS:

I. Structure, properties, and occupational exposure limits for the selected flavoring chemicals Page S3

II. Demographics of the study participants Page S4


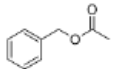

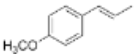
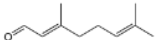
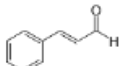

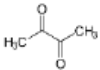

III. E-cigarette use patterns of the 23 subjects in our study Page S4

IV. The detailed experimental conditions Page S5

V. Calibration curve for 2OHTA Page S5

I. Structure, properties, and occupational exposure limits for the selected flavoring chemicals

Table S1. Characteristics of flavoring chemicals

Name	Flavor	Structure	Property	Occupational exposure limits (mg/m ³)					
				OSHA PEL		ACGIH TLV		NIOSH REL	
				TWA	STEL	TWA	STEL	TWA	STEL
Benzyl alcohol	Fruity		MW: 108.14 g/mol BP: 205.3 °C, VP: 0.18 kPa						
Benzyl acetate	Fruity		MW: 150.18 g/mol BP: 212 °C, VP: 0.02 kPa	61		61			
Ethyl acetate	Fruity		MW: 88.11 g/mol BP: 77.1 °C, VP: 9.7 kPa	1400		1400		1400	7200
Anethole	Sweet		MW: 148.21 g/mol BP: 234 °C, VP: > 1 Pa						
Citral	Citrus		MW: 152.24 g/mol BP: 229 °C, VP: 13.3 Pa			31 (dermal)			
Cinnamaldehyde	Spicy, sweet		MW: 132.16 g/mol BP: 248 °C, VP: > 1 Pa						
Vanillin	Sweet, Fatty		MW: 152.15 g/mol BP: 285 °C, VP: > 1 Pa						
2,3-butanedione (diacetyl)	Fatty, Buttery		MW: 86.09 g/mol BP: 88 °C, VP: 7.57 kPa			0.035	0.070	0.018	0.088
2,3-pentanedione (Acetylpropionyl)	Fatty, Buttery		MW: 100.12 g/mol BP: 109.9 °C, VP: 2.67 kPa					0.038	0.127

II. Demographics of the study participants

The demographics of the study participants are summarized in Table S2.

Table S2. Summary of the study participants

Number of subjects	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

III. E-cigarette use patterns of the 23 subjects in our study

Table S3 shows the mean, the standard deviation, and the range of e-cigarette vaping topography, device power output, and nicotine contents of the 23 subjects 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 VG-based E-liquids (14 out of 23 subjects), followed by PG:VG mixed E-liquid (7 subjects), and PG-based E-liquid (2 subjects).

Table S3. E-cigarette vaping patterns from the study subjects (N = 23)

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

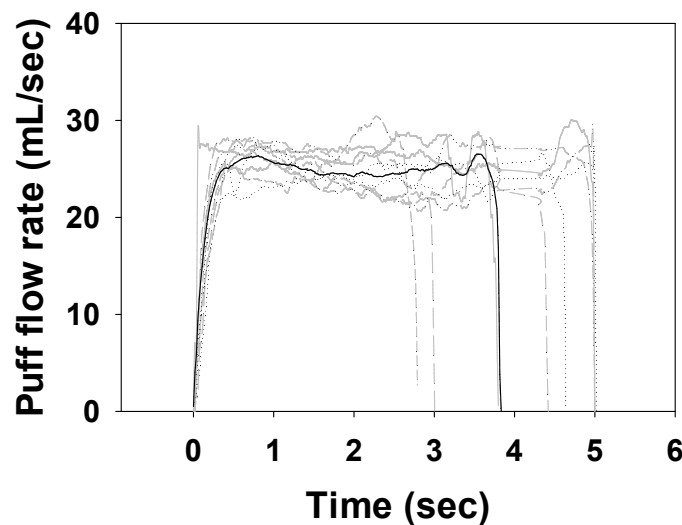


Figure S1. E-cigarette vaping topography observed using the Cress pocket device from 23 subjects

IV. The detailed experimental conditions

The e-vapor generation conditions are tabulated in Table S4.

Table S4. The experimental factors used in the experiments

Experiments	Factors	Settings	Other Settings for Particle Generation
Device setting	Device power (watt)	6.4, 31.3	90 mL puff volume, 3.8 sec puff duration, 12 mg/ml nicotine in VG
	Air hole size (mm)	1, 1.5, 2	
Vaping topography	Puff volume (mL)	35, 90, 170	6.4W, 2 mm air hole and 12 mg/ml nicotine in VG;
	Puff duration (sec)	2, 3.8	
E-liquid base material	Base material	PG, VG, PG&VG (v:v = 1:1)	6.4W, 2 mm air hole, 90 mL puff volume, 3.8 sec puff duration
	Nicotine (mg/ml)	12	
E-liquid flavoring ingredients	Flavor	8 flavors*	6.4W, 2 mm air hole, 90 mL puff volume, 3.8 sec puff duration, VG
	Flavoring level (%)	1 and 10% by volume**	

* Strawberry (Ripe), Dragonfruit, Menthol, Cinnamon, Bubblegum, Bavarian cream, Sweet cream and Graham cracker; ** 0.1 and 1% for cinnamon flavor

V. Calibration curve for 2OHTA

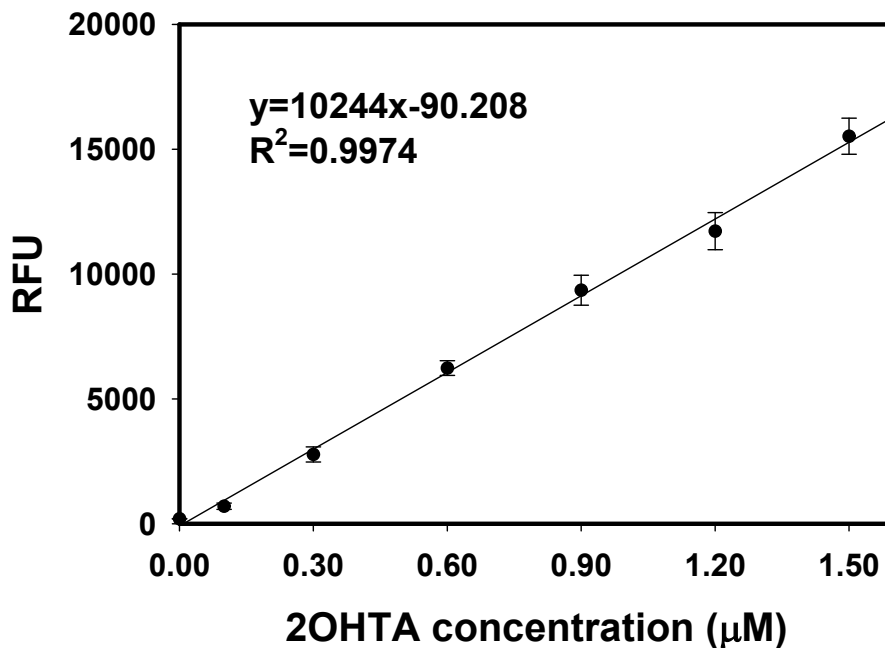


Figure S2. Calibration curve for 2OHTA