

SUPPLEMENTAL MATERIALS

LC-HRMS

LC-HRMS systems consisted of a Thermo Q-Exactive mass spectrometer coupled to a Thermo Vanquish Horizon-Class liquid chromatograph with an autosampler and heated column compartment. The separation was performed using a Waters BEH C18 (2.1 x 100 mm, 1.7 μ m) column.

Table S1a Liquid Chromatographic Conditions

Column Compartment	
Column	Acquity UPLC BEH C18 1.7 μ m 2.1 x 100 mm
Guard column	Acquity UPLC BEH C18 VanGuard Pre-column, 130Å, 1.7 μ m, 2.1 mm X 5 mm
Column Temp	50 °C
Auto Sampler	
Wash Mode	Both
Wash Speed	50.0 μ L/sec
Wash Time	2 sec
Dispense Speed	10.0 μ L/sec
Draw Speed	0.666 μ L/sec
Injection Volume	0.1 μ L
Sample Temp	10 °C
Pump Solvents	
Needle Wash	1:1:1:1 Water:Methanol:Acetonitrile:Isopropanol
Seal Wash	75:25 Isopropanol:Water
Mobile Phase A1	5 mM Ammonium Acetate, pH 8.5
Mobile Phase B1	Methanol

Table S1b Liquid Chromatographic Conditions

Mobile Phase Gradient				
Time (min)	%A	%B	Flow Rate (mL/min)	Curve
0.00	95	5	0.200	5
20.00	20	80	0.200	5
22.00	20	80	0.200	5

22.01	95	5	0.200	5
26.00	95	5	0.200	5

Q-Exactive Mass Spectrometer

Table S2a. Spectrometer Parameters

Acquisition Mode	Full Scan and ddMS ²
Sheath Gas Flow Rate	50
Aux Gas Flow Rate	15
Sweep Gas Flow Rate	5
Spray Voltage	3,500 V
Mass/Charge Range	60-800
Capillary temp	320 °C
S-Lens RF Level	50.0
Aux gas heater temp	250 °C

Table S2b. Mass Spectrometer parameters for full scan acquisition

Acquisition Mode	Full Scan
Tune File	pos_ESI_rev1
Divert valve	2 min to 23 min
Chrom peak width	5 sec
Run Time	2 min to 23 min
Polarity	Positive
In Source CID	0 V
Micro-scans	1
Resolution	140,000
AGC Target	1E6
Max IT	400 ms
Number of Scan Ranges	1
Scan Range	60 to 800 m/z
Spectrum Data Type	Profile

Table S2c. Mass Spectrometer parameters for data dependent ddMS² scan acquisition

Acquisition Mode	Full Scan→ddMS ²
Tune File	pos_ESI_rev1*
User Role	Advanced
Divert valve	2 min to 23 min
Chrom. Peak width	5 sec

Run Time	2 min to 23 min
Polarity	Positive
In Source CID	0 V
Full MS	
Micro-scans	1
Resolution	70,000
AGC Target	3E6
Max IT	100 ms
Number of Scan Ranges	1
Scan Range	60 to 800 m/z
Spectrum Data Type	Profile
dd-MS ²	
Micro-scans	1
Resolution	17,500
AGC Target	1E5
Max IT	150 ms
Loop Count	10
MSX	1
Isolation Window	1.2 m/z
Isolation Offset	0
NCE/Stepped	NCE: 25, 50, 75
Spectrum Data Type	Profile
dd-Setting	
Min AGC target	1E3
Intensity Threshold	6.7E3
Exclude Isotopes	On
Dynamic Exclusion	10.0 sec

GC-MS

GC-MS systems consisted of an Agilent 7890GC/5977MSD gas chromatograph equipped with an electron ionization (EI) source. The separation was performed using a Restek Stabilwax (30m x 0.25mm x 0.25µm) column with a Restek (5 meter) integra guard column. All GC-MS NTA data were collected by Altria Client Services, LLC. using their validated and it is published method [8].

Table S3a. Gas Chromatograph Parameters

Column	Stabilwax 30m x 0.25mm x 0.25µm
Injection Volume	1 µL
Inlet Temp	260°C
Inlet Mode	Split (5:1)
Flow Control Mode	Constant Flow
Column Flow	1.2 mL/min
Transfer Line Temp	260°C
Oven Program	

Initial Temp	60°C – Hold 1.25 min
Ramp 1	15°C/min to 210°C – Hold 2 min
Ramp 2	30°C/min to 260°C – Hold 9 min
Analysis Time	23.92 min

Table S3b. Mass Spectrometer Parameters

Acquisition Mode	Scan
Tune File	etune.u
Solvent Delay	2.90 min
EMV Mode	Gain Factor
Gain Factor	2.00
Mass Range	35-450
Threshold	100
Sample #	2
MS Source Temp	230°C
MS Quad Temp	150°C

Table S4 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
3.72	Decamethylcyclopentasiloxane Isomer 3	541-02-6	CONFIRMED	ND	ND	ND	12.6	ND	ND	ND	ND	ND	12.6	0.0	3	E&L
4.08	Pyridine	110-86-1	CONFIRMED	ND	ND	ND	1.6	1.2	1.0	ND	ND	ND	1.2	0.3	1	Flavorant
4.14	1,8-Cineole	470-82-6	HIGH	0.7	0.8	0.8	0.9	0.7	ND	0.7	ND	ND	0.8	0.1	1	Flavorant
5.04	Hydroxyacetone	116-09-6	CONFIRMED	8.1	9.1	10.2	15.8	9.6	8.3	10.0	9.1	8.8	9.9	2.3	4	dehydration of glycerol and/or oxidation of PG
5.32	Dodecamethylcyclohexasiloxane Isomer 1	540-97-6	HIGH	23.8	23.2	24.1	31.8	26.0	13.0	19.1	10.3	15.6	20.8	6.8	3	E&L
6.50	Acetic acid	64-19-7	CONFIRMED	16.6	8.3	9.0	9.3	5.5	8.1	ND	ND	8.2	9.3	3.4	1	Flavorant
6.60	2-ethyl-1-hexanol	104-76-7	CONFIRMED	0.7	0.8	0.7	ND	ND	ND	0.8	ND	0.7	0.8	0.0	3	E&L
6.63	Menthone	89-80-5	CONFIRMED	21.9	24.0	22.7	25.7	22.5	18.8	22.1	20.2	20.5	22.0	2.1	4	oxidized menthol
6.70	Menthofuran	494-90-6	CONFIRMED	1.2	1.4	1.3	1.6	1.3	1.0	1.3	1.2	1.2	1.3	0.2	1	Flavorant
6.79	Isomenthone	491-07-6	CONFIRMED	6.9	7.3	7.1	8.0	7.0	5.7	6.8	6.2	6.1	6.8	0.7	1	Flavorant
6.80	Tetradecamethylcycloheptasiloxane	107-50-6	CONFIRMED	ND	ND	8.5	8.9	ND	ND	ND	ND	ND	8.7	0.3	3	E&L
7.07	1,3Dioxolane-2methanol_2,4dimethyl-Iso1	53951-43-2	MEDIUM	2.7	3.2	3.1	3.6	3.1	2.5	2.0	1.8	1.9	2.6	0.6	4	PG degradant
7.20	Linalool	78-70-6	CONFIRMED	1.0	1.1	1.0	1.2	1.1	0.8	1.1	0.9	1.0	1.0	0.1	1	Flavorant
7.31	Linalyl acetate	115-95-7	CONFIRMED	1.5	1.6	1.5	1.7	1.5	1.3	1.5	1.3	1.5	1.5	0.1	1	Flavorant
7.40	Menthyl acetate	89-48-5	CONFIRMED	3.6	3.8	3.7	4.2	3.7	3.1	3.7	3.3	3.3	3.6	0.3	1	Flavorant
7.56	1,3-Dioxolane-4-methanol_2,2-dimethyl-	100-79-8	CONFIRMED	47.8	62.4	35.6	66.6	53.0	34.5	5.5	4.9	9.0	35.5	24.2	4	VG degradant
7.60	Isopulegol Isomer	7786-67-6	CONFIRMED	ND	0.8	ND	0.8	0.8	ND	ND	ND	ND	0.8	0.0	4	reduction of isopulegone
7.68	Ethanone_1-(2-pyridinyl)-	1122-62-9	CONFIRMED	17.0	19.3	18.9	21.6	18.2	15.0	18.0	15.6	17.0	17.8	2.0	1	Flavorant
7.78	Terpinen-4-ol	562-74-3	CONFIRMED	1.0	1.3	ND	1.1	ND	ND	1.1	ND	ND	1.1	0.1	1	Flavorant
7.80	Unknown Menthol Related Comp (RRT 0.520)	NA	NA	4.2	5.3	5.9	8.7	4.7	4.9	5.7	6.3	4.4	5.6	1.4	4	Menthol (Flavorant) reaction

Table S4 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
7.91	Acetylpyrazine	22047-25-2	CONFIRMED	2.1	2.4	2.3	2.6	2.1	1.9	2.2	1.8	2.2	2.2	0.2	1	Flavorant
8.24	Lavandulol	498-16-8	CONFIRMED	2.6	3.0	3.0	3.0	2.2	2.0	2.3	2.1	2.4	2.5	0.4	1	Flavorant
8.20	5-Methyl-2-(1-methylethyl)-Cyclohexanol	1490-04-6	CONFIRMED	4.1	5.0	4.3	5.6	4.7	3.6	4.7	3.4	4.0	4.4	0.7	1	Isomer of menthol (Flavorant)
8.21	Pulegone	89-82-7	CONFIRMED	2.5	3.0	3.1	2.2	3.1	2.5	2.7	2.5	2.8	2.7	0.3	1	Flavorant
8.31	Hexadecamethylcyclooctasil oxane	556-68-3	CONFIRMED	1.7	1.5	2.9	3.4	1.4	ND	1.3	ND	1.3	1.9	0.9	3	E&L
8.45	Diethoxydimethylsilane	78-62-6	CONFIRMED	ND	ND	ND	ND	ND	ND	ND	0.8	ND	0.8	0.0	3	E&L
8.47	Terpinyl propionate	80-27-3	MEDIUM	0.8	1.6	1.1	1.2	1.0	0.8	0.9	1.2	1.2	1.1	0.3	1	Flavorant
8.47	Unknown (RRT 0.559)	NA	NA	ND	ND	ND	1.0	ND	ND	0.9	ND	0.8	0.9	0.1	5	NR
8.56	Borneol	464-45-9	CONFIRMED	ND	0.7	ND	ND	ND	ND	ND	ND	ND	0.7	0.0	4	α-pinene protonation, capture of this carbocation by H2O accompanied by rearrangement of bicyclo carbon skeleton
8.66	Nicotinealdehyde	500-22-1	CONFIRMED	1.2	1.0	1.0	1.1	1.0	0.8	1.0	0.8	0.9	1.0	0.1	4	demethylation of 3-acetylpyridine
8.80	Piperitone	89-81-6	CONFIRMED	ND	ND	0.7	0.8	ND	ND	ND	ND	ND	0.8	0.0	1	Flavorant
9.36	Dipropylene glycol	110-98-5	CONFIRMED	39.0	42.6	42.0	ND	40.5	33.8	39.8	35.5	37.7	38.8	3.1	4	PG degradant
9.40	beta-Damascenone	23726-93-4	CONFIRMED	3.6	4.0	3.9	4.4	3.8	3.1	3.7	3.3	3.5	3.7	0.4	1	Flavorant
9.50	Octadecamethylcyclononasiloxane	556-71-8	CONFIRMED	ND	ND	ND	0.8	ND	ND	ND	ND	ND	0.8	0.0	3	E&L
9.52	N,2,3-trimethyl-2-isopropylbutamide	51115-67-4	CONFIRMED	77.0	87.4	83.3	99.0	83.0	69.2	81.3	73.4	77.4	81.2	8.7	1	Flavorant
9.61	(Z)-beta-damascone	23726-92-3	CONFIRMED	14.5	15.2	15.7	33.3	15.5	12.9	15.3	13.6	14.5	16.7	6.3	1	Flavorant
9.95	2-(4-methoxyphenyl)1-pyrroline	NA	MEDIUM	3.0	2.6	2.6	2.7	2.4	1.9	3.1	2.3	2.4	2.6	0.4	4	Nicotine degradant
10.53	N-methyl-4-(3-pyridyl)-3-buten-1-amine	15585-43-0	HIGH	2.6	2.8	2.8	2.9	2.6	2.1	2.5	2.3	2.4	2.5	0.3	4	Nicotine degradant

Table S4 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stddev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
10.55	N-Methylanabasine	24380-92-5	CONFIRMED	1.7	2.0	1.9	2.1	1.8	1.5	1.8	1.6	1.7	1.8	0.2	4	Nicotine degradant
10.55	Phenol	108-95-2	CONFIRMED	0.9	1.0	1.0	1.7	1.0	1.1	1.1	1.2	1.1	1.1	0.2	2	HPHC
11.10	Unknown (RRT 0.724)	NA	NA	3.1	3.5	3.7	3.8	3.8	4.1	4.0	3.7	4.1	3.7	0.3	5	NR
11.26	Triacetin	102-76-1	CONFIRMED	ND	2.2	ND	ND	ND	ND	1.1	ND	ND	1.6	0.8	4	acetic acid + glycerol
11.30	Unknown Nic Related Comp.(RRT 0.743)	NA	NA	1.7	1.2	ND	ND	ND	ND	ND	0.9	0.8	1.2	0.4	4	Nicotine degradant
12.30	Piperonal	120-57-0	CONFIRMED	2.5	2.9	2.7	3.3	2.7	2.2	2.6	2.3	2.6	2.6	0.3	1	Flavorant
12.70	Unknown Nic.Related Comp.(RRT 0.840)	NA	NA	9.1	2.9	3.0	3.1	2.8	ND	2.2	1.1	1.6	3.2	2.5	4	Nicotine degradant
12.70	3-(1,3-dimethylpyrrol-2-yl)pyridine	78210-38-5	CONFIRMED	3.2	2.7	3.1	2.9	2.5	2.4	2.5	2.4	2.3	2.6	0.3	4	Nicotine degradant
13.57	Unknown Nic.Related Comp.(RRT 0.849)	NA	NA	2.8	ND	2.7	3.1	2.9	2.5	3.1	2.6	3.0	2.8	0.2	4	Nicotine degradant
13.90	3-(1,3-dimethylpyrrol-2-yl)pyridine Iso	78210-38-5	HIGH	2.1	2.0	2.1	2.5	2.0	1.8	1.9	2.0	2.0	2.0	0.2	4	Nicotine degradant
13.99	2-hydroxypropyl benzoate	37086-84-3	CONFIRMED	6.5	7.7	8.1	8.9	7.6	6.2	6.5	6.6	6.5	7.2	0.9	4	benzoic acid + PG (esterification)
14.31	1,3-Ethoxyethylideneglycerol	NA	MEDIUM	2.0	4.1	1.1	4.2	4.1	ND	ND	3.0	3.1	3.1	1.2	4	VG degradant
14.41	Unknown Nic.Related Comp.(RRT 0.956)	NA	NA	ND	1.5	ND	ND	ND	ND	ND	ND	ND	1.5	0.0	4	Nicotine degradant
14.53	p-Dioxane-2,5-dimethanol	14236-12-5	CONFIRMED	13.7	15.0	14.0	14.9	13.8	11.7	13.7	12.3	12.3	13.5	1.2	4	2VG dehydration
14.60	Unknown Nic.Related Comp.(RRT 0.970)	NA	NA	4.3	6.3	3.9	4.3	4.6	3.8	4.5	3.6	3.7	4.3	0.8	4	Nicotine degradant
14.66	N-Propylnormicotine	91907-45-8	CONFIRMED	2.0	1.7	2.2	1.7	1.4	1.2	1.3	1.2	ND	1.6	0.4	4	Nicotine degradant
14.70	Bis(2,6-hydroxymethyl)dioxane	54120-69-3	CONFIRMED	31.5	34.7	33.5	54.1	48.6	41.9	32.6	31.6	45.2	39.3	8.4	4	2VG dehydration
14.72	Bis(2,6-hydroxymethyl)dioxane - Iso2	54120-69-3	HIGH	5.8	14.4	7.5	71.9	8.4	6.7	6.1	6.5	67.3	21.6	27.3	4	2VG dehydration
14.89	Bis(2,6-hydroxymethyl)dioxane - Iso3	54120-69-3	HIGH	217.8	24.6	59.3	36.2	25.1	22.2	22.2	21.2	70.6	55.5	63.5	4	2VG dehydration
15.00	Bis(2,6-hydroxymethyl)dioxane - Iso4	54120-69-3	HIGH	27.5	28.5	28.4	31.9	28.9	24.2	27.8	25.9	26.5	27.7	2.2	4	2VG dehydration
15.19	Unknown Nic.Related Comp.(RRT 1.012)	NA	NA	2.5	3.3	2.8	3.8	2.7	2.6	2.4	2.9	2.4	2.8	0.5	4	Nicotine degradant
15.20	Bis(2,6-hydroxymethyl)dioxane - Iso5	54120-69-3	HIGH	10.0	10.8	11.0	11.7	10.4	8.6	10.0	9.6	10.0	10.2	0.9	4	2VG dehydration
16.50	Unknown Nic. Related Comp. (RRT 1.098)	NA	NA	ND	ND	ND	ND	ND	ND	2.1	ND	1.5	1.8	0.4	4	Nicotine degradant

Table S4 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
16.80	Hexadecanoic Acid	57-10-3	CONFIRMED	6.2	3.5	1.9	3.7	1.0	3.4	2.2	1.6	0.7	2.7	1.7	3	E&L
17.36	Phenol_2-(1-phenylethyl)-	4237-44-9	CONFIRMED	ND	ND	ND	ND	ND	1.4	ND	ND	ND	1.4	0.0	4	Phenylethanol (from phenylethyl acetate) + phenol
17.50	2-(beta nicotyrine)propan-2-one Iso-1 ^a	2416242-88-9	HIGH	7.2	5.9	6.4	6.4	6.6	5.7	6.2	6.0	5.4	6.2	0.5	4	Nicotine degradant
19.08	Caffeine	58-08-2	CONFIRMED	13.7	14.3	14.3	16.0	14.6	12.3	14.4	12.9	13.2	14.0	1.1	1	Flavorant
19.80	1-(beta nicotyrine)propan-2-one Iso-2 ^a	2416242-88-9	HIGH	15.5	13.1	14.6	14.4	14.6	12.8	14.3	14.1	12.8	14.0	0.9	4	Nicotine degradant

^a1-(beta nicotyrine)propan-2-one: 1-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)propan-2-one

^a2-(beta nicotyrine)acetaldehyde: 2-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)acetaldehyde

Table S5 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
4.08	Pyridine	110-86-1	CONFIRMED	1.3	1.0	0.9	1.0	1.1	1.0	1.2	ND	1.2	1.1	0.1	1	Flavorant
5.04	Hydroxyacetone	116-09-6	CONFIRMED	8.2	6.8	6.5	7.3	6.9	ND	8.3	8.2	7.9	7.5	0.7	4	dehydration of glycerol and/or oxidation of PG
5.32	Dodecamethylcyclhexasiloxane Isomer 1	540-97-6	HIGH	18.0	15.6	15.3	17.4	17.1	17.6	18.6	17.4	17.3	17.1	1.1	3	E&L
5.61	1-((ethoxydimethylsilyl)oxy)propan-2-ol	NA	MEDIUM	1.2	1.1	1.0	0.9	1.0	1.0	1.0	0.9	0.9	1.0	0.1	4	hydrolysis of E&L source compound (such as dodecamethylcyclhexasiloxane)
6.50	Acetic acid	64-19-7	CONFIRMED	17.7	8.5	9.2	9.4	9.6	12.1	10.9	9.5	14.9	11.3	3.1	1	Flavorant
6.60	2-ethyl-1-hexanol	104-76-7	CONFIRMED	0.9	ND	ND	0.9	ND	ND	ND	ND	ND	0.9	0.0	3	E&L
6.63	Menthone	89-80-5	CONFIRMED	18.1	15.9	17.0	17.6	16.5	17.4	18.9	18.0	18.5	17.5	1.0	4	oxidized menthol
6.70	Menthofuran	494-90-6	CONFIRMED	1.0	ND	ND	0.9	0.9	ND	1.0	1.0	1.0	0.9	0.0	1	Flavorant

Table S5 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
6.79	Isomenthone	491-07-6	CONFIRMED	5.8	5.1	5.4	5.5	5.3	5.5	6.0	5.6	5.8	5.5	0.3	1	Flavorant
7.07	1,3Dioxolane-2methanol_2,4dimethyl-Iso1	53951-43-2	MEDIUM	2.7	2.2	2.2	2.5	2.3	2.6	1.9	1.7	1.9	2.2	0.3	4	PG degradant
7.20	1,3Dioxolane-2methanol_2,4dimethyl-Iso2	53951-43-2	MEDIUM	1.4	ND	ND	ND	ND	ND	ND	ND	ND	1.4	0.0	4	PG degradant
7.20	Linalool	78-70-6	CONFIRMED	1.0	ND	ND	0.9	ND	0.9	0.9	0.9	0.9	0.9	0.0	1	Flavorant
7.31	Linalyl acetate	115-95-7	CONFIRMED	1.3	1.0	1.2	1.3	1.2	1.2	1.3	1.3	1.4	1.2	0.1	1	Flavorant
7.40	Menthyl acetate	89-48-5	CONFIRMED	2.9	2.6	2.8	3.0	2.6	2.8	3.2	3.0	3.1	2.9	0.2	1	Flavorant
7.50	Unknown Menthol Related Comp.(RRT 0.503)	NA	NA	1.2	2.7	2.1	2.2	2.0	1.8	1.2	2.2	1.6	1.9	0.5	4	Menthol (Flavorant) reaction
7.56	1,3-Dioxolane-4-methanol_2,2-dimethyl-	100-79-8	CONFIRMED	13.0	9.3	10.7	11.5	11.9	11.6	7.6	6.1	7.2	9.9	2.4	4	VG degradant
7.68	Ethanone_1-(2-pyridinyl)-	1122-62-9	CONFIRMED	18.2	14.8	15.5	17.5	16.5	16.9	18.0	17.3	17.1	16.9	1.1	1	Flavorant
7.71	Unknown Menthol Related Comp.(RRT 0.523)	NA	NA	0.9	0.9	0.9	0.9	0.9	0.9	0.9	1.0	1.0	0.9	0.0	4	Menthol (Flavorant) reaction
7.78	Terpinen-4-ol	562-74-3	CONFIRMED	1.1	0.9	ND	1.0	ND	1.2	0.9	0.9	ND	1.0	0.1	1	Flavorant
7.91	Acetylpyrazine	22047-25-2	CONFIRMED	2.1	ND	1.8	1.7	ND	2.0	2.0	ND	ND	1.9	0.1	1	Flavorant
8.00	Methyl benzoate	93-58-3	CONFIRMED	4.4	3.6	ND	2.6	3.3	ND	4.1	4.1	4.7	3.8	0.7	4	benzoic acid + MeOH
8.24	Lavandulol	498-16-8	CONFIRMED	2.3	2.1	2.1	2.4	2.1	2.3	2.2	2.5	2.6	2.3	0.2	1	Flavorant
8.20	5-Methyl-2-(1-methylethyl)-Cyclohexanol	1490-04-6	CONFIRMED	4.6	3.8	3.8	4.1	3.6	4.5	4.8	4.4	3.4	4.1	0.5	1	Isomer of menthol (Flavorant)
8.21	Pulegone	89-82-7	CONFIRMED	1.7	1.6	1.8	2.0	1.8	1.8	2.0	2.0	1.7	1.8	0.1	1	Flavorant
8.31	Hexadecamethylcyclooctasiloxane	556-68-3	CONFIRMED	1.7	2.2	1.8	1.6	1.8	1.5	1.5	1.5	1.5	1.7	0.2	3	E&L
8.45	Diethoxydimethylsilane	78-62-6	CONFIRMED	4.4	5.1	4.6	4.0	4.2	3.7	3.9	4.2	4.3	4.3	0.4	3	E&L
8.47	1,3-Dioxolane_4-methyl-2-pentyl-	1599-49-1	LOW	2.9	2.5	2.5	2.9	2.5	2.6	2.0	1.9	ND	2.5	0.4	4	PG + hexanal
8.47	Terpinyl propionate	80-27-3	MEDIUM	0.9	ND	ND	1.0	ND	0.9	1.0	0.9	0.9	0.9	0.1	1	Flavorant

Table S5 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
8.66	Nicotinealdehyde	500-22-1	CONFIRMED	1.0	0.9	ND	0.9	0.9	0.9	1.0	0.9	ND	0.9	0.0	4	demethylation of 3-acetylpyridine
9.36	Dipropylene glycol	110-98-5	CONFIRMED	46.6	38.0	39.7	44.1	41.9	43.4	44.5	43.2	43.3	42.7	2.6	4	2PG - H2O
9.46	Benzaldehyde_2,3-dimethyl-	5779-93-1	MEDIUM	1.6	1.2	ND	1.2	ND	1.4	1.5	1.5	1.4	1.4	0.2	3	E&L
9.50	Benzyl alcohol	100-51-6	CONFIRMED	40.0	33.6	35.0	39.6	36.9	38.3	39.0	38.4	38.2	37.7	2.1	1	Flavorant
9.52	N,2,3-trimethyl-2-isopropylbutamide	51115-67-4	CONFIRMED	78.3	65.7	68.4	74.7	70.5	74.2	76.4	74.6	74.7	73.1	4.0	1	Flavorant
9.61	(Z)-beta-damascone	23726-92-3	CONFIRMED	13.7	11.6	12.3	13.2	12.3	14.3	14.2	13.6	13.5	13.2	0.9	1	Flavorant
9.95	2-(4-methoxyphenyl)-1-pyrroline	NA	MEDIUM	3.3	3.4	3.8	3.7	3.8	2.7	3.3	3.7	3.8	3.5	0.4	4	Nicotine degradant
10.53	N-methyl-4-(3-pyridyl)-3-buten-1-amine	15585-43-0	HIGH	2.7	2.3	2.4	2.4	2.3	2.5	2.4	2.3	2.2	2.4	0.1	4	Nicotine degradant
10.55	N-Methylanabasine	24380-92-5	CONFIRMED	2.0	1.7	1.7	1.9	1.8	1.9	1.9	1.9	1.8	1.8	0.1	4	Nicotine degradant
10.55	Phenol	108-95-2	CONFIRMED	1.4	1.1	1.1	1.2	1.2	1.2	1.5	1.4	1.5	1.3	0.2	2	HPHC
11.20	Dihydroxyacetone	96-26-4	CONFIRMED	1.3	1.2	1.1	1.4	1.1	1.2	1.2	1.2	ND	1.2	0.1	4	Oxidation of glycerol
12.30	Piperonal	120-57-0	CONFIRMED	2.4	2.0	2.1	2.4	2.4	2.4	2.5	2.4	2.4	2.3	0.2	1	Flavorant
12.35	Glyceryl monoacetate	106-61-6	CONFIRMED	15.8	11.8	14.2	14.1	15.4	14.3	14.2	14.9	14.9	14.4	1.1	4	VG esterification/transesterification
12.70	3-(1,3-dimethylpyrrol-2-yl)pyridine	78210-38-5	CONFIRMED	2.8	2.9	2.5	2.6	2.3	2.6	2.5	2.0	1.9	2.5	0.3	4	Nicotine degradant
13.57	Unknown Nic. Related Comp.(RRT 0.849)	NA	NA	3.7	4.3	2.8	7.2	2.9	ND	3.3	3.4	5.2	4.1	1.5	4	Nicotine degradant
13.81	Unknown Nic.Related Comp.(RRT 0.923)A	NA	NA	1.4	1.3	1.4	1.3	1.5	1.0	0.9	1.3	1.3	1.3	0.2	4	Nicotine degradant
14.31	1,3-Ethoxyethylideneglycerol	NA	MEDIUM	5.5	3.9	3.9	4.9	4.1	1.6	4.0	4.7	4.2	4.1	1.1	4	VG degradant
14.53	p-Dioxane-2,5-dimethanol	14236-12-5	CONFIRMED	14.0	11.7	12.6	13.7	13.2	13.7	14.3	13.6	13.7	13.4	0.8	4	2VG dehydration
14.60	Unknown Nic.Related Comp.(RRT 0.970)	NA	NA	5.8	3.1	4.0	4.2	4.4	4.8	4.2	4.9	4.5	4.4	0.7	4	Nicotine degradant
14.66	N-Propylnormicotine	91907-45-8	CONFIRMED	1.3	ND	ND	ND	1.2	1.1	1.3	ND	ND	1.2	0.1	4	Nicotine degradant

Table S5 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
14.70	Bis(2,6-hydroxymethyl) dioxane	54120-69-3	CONFIRMED	53.4	44.0	46.5	50.7	48.5	51.3	52.8	51.9	50.2	49.9	3.1	4	2VG dehydration
14.72	Bis(2,6 hydroxymethyl) dioxane - Iso2	54120-69-3	HIGH	39.4	28.3	ND	36.8	ND	48.7	38.2	42.4	33.8	38.2	6.4	4	2VG dehydration
14.89	Bis(2,6-hydroxymethyl) dioxane - Iso3	54120-69-3	HIGH	29.6	24.0	21.6	24.7	24.8	23.0	26.2	29.4	26.9	25.6	2.7	4	2VG dehydration
15.00	Bis(2,6-hydroxymethyl) dioxane - Iso4	54120-69-3	HIGH	31.6	25.1	27.5	29.0	27.8	26.7	29.9	29.5	28.5	28.4	1.9	4	2VG dehydration
15.19	Unknown Nic.Related Comp.(RRT 1.012)	NA	NA	3.5	4.8	3.5	6.5	2.6	5.0	5.0	3.4	4.3	4.3	1.2	4	Nicotine degradant
15.20	Bis(2,6-hydroxymethyl) dioxane - Iso5	54120-69-3	HIGH	12.0	10.0	11.5	11.6	11.1	11.8	12.0	12.4	11.7	11.5	0.7	4	2VG dehydration
16.80	Hexadecanoic Acid	57-10-3	CONFIRMED	21.7	10.0	14.3	15.0	10.2	10.0	7.7	8.2	6.3	11.5	4.8	3	E&L
17.00	2-(beta nicotyrine)acetaldehyde Iso-1 ^a	NA	MEDIUM	ND	0.9	ND	1.1	ND	1.5	1.3	ND	ND	1.2	0.3	4	Nicotine degradant
17.50	1-(beta nicotyrine)propan-2-one Iso-1 ^a	24162-42-88-9	HIGH	5.6	5.6	5.4	6.2	5.7	6.7	5.4	5.2	4.8	5.6	0.5	4	Nicotine degradant
18.56	2-(beta nicotyrine)acetaldehyde Iso-2 ^a	NA	MEDIUM	1.2	1.0	1.3	1.7	1.4	2.0	2.0	1.3	1.2	1.5	0.4	4	Nicotine degradant
19.08	Caffeine	58-08-2	CONFIRMED	15.5	12.4	13.3	14.4	14.0	14.2	15.1	15.0	14.5	14.2	1.0	1	Flavorant
19.80	1-(beta nicotyrine)propan-2-one Iso-2 ^b	24162-42-88-9	HIGH	12.8	12.8	12.9	15.1	14.5	16.4	12.6	13.1	12.0	13.6	1.4	4	Nicotine degradant
22.53	Unknown Long Chain Alkane (RRT 1.482)	NA	NA	ND	17.0	ND	ND	ND	ND	ND	ND	ND	17.0	0.0	5	NR

^a 1-(beta nicotyrine)propan-2-one: 1-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)propan-2-one

^a 2-(beta nicotyrine)acetaldehyde: 2-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)acetaldehyde

Table S6 LC-HRMS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

RT [min]	RRT	Name	CAS #	Confidence Level	Estimated Amount µg/g									Avg (µg/g)	Stdev	P-Value	Group	Rationalization
					Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B							
					Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3					
2.07	0.15	unknown PG_VG related compound RRT 0.16 ^a	NA	NA	7.8	6.0	8.5	9.3	8.7	7.5	7.5	9.1	9.9	8.3	1.2	1.2E-13	4	dehydration of PG VG to form conjugate
2.40	0.17	hydroxyacetone	116-09-6	high	10.5	11.4	11.5	12.8	11.8	9.9	11.9	11.9	12.6	11.6	0.9	3.6E-15	4	dehydration of glycerol and/or oxidation of PG
2.84	0.21	4- methoxybenzaldehyde	123-11-5	high	3.5	3.6	3.9	4.1	4.1	3.5	4.4	4.3	4.8	4.0	0.4	2.8E-15	4	methoxylated benzaldehyde
3.25	0.24	unknown nicotine related compound RRT 0.24	NA	NA	36.3	31.7	32.0	37.3	37.6	45.5	37.4	32.3	36.3	36.3	4.2	3.0E-04	4	nicotine degradant
4.43	0.32	theobromine	83-67-0	high	ND	1.9	2.8	3.2	3.0	2.7	3.3	3.2	3.4	2.9	0.5	NA	1	Flavorant
7.21	0.52	caffeine	58-08-2	confirmed	5.3	5.6	5.5	6.3	6.1	5.5	6.0	5.7	6.3	5.8	0.4	NA	1	Flavorant
10.24	0.74	2,3-dihydroxypropyl benzoate	3376-59-8	high	28.9	36.9	39.7	58.3	35.0	33.8	42.3	52.2	34.7	40.2	9.4	1.5E-12	4	benzoic acid + VG
11.58	0.84	N-methylmyosmine	525-74-6	high	18.2	28.8	27.8	31.7	18.3	28.0	19.4	27.4	35.0	26.1	6.1	5.9E-06	4	nicotine degradant
11.78	0.85	1-(1-methyl-5- (pyridin-3-yl)-1H- pyrrol-2-yl)propan-2- one isomer 1	2416242- 88-9	high	7.3	6.2	7.0	6.7	7.3	6.4	7.4	7.6	7.2	7.0	0.5	5.5E-17	4	nicotine degradant
12.43	0.90	1-(1-methyl-5- (pyridin-3-yl)-1H- pyrrol-2-yl)propan-2- one isomer 2	2416242- 88-9	high	10.6	9.2	10.4	9.7	10.3	9.1	10.6	11.3	10.5	10.2	0.7	1.5E-17	4	nicotine degradant
13.42	0.97	unknown benzyl alcohol related compound RRT 0.97	NA	NA	13.6	15.2	14.9	16.4	15.4	12.8	15.5	15.3	16.5	15.1	1.2	2.1E-16	4	methoxylated, oxidized and ring opening of benzyl alcohol
16.26	1.18	2-isopropyl-N, 2, 3- trimethylbutylbutamide	51115-67-4	high	79.6	90.2	88.7	93.8	87.4	74.1	89.1	90.8	99.2	88.1	7.4	7.4E-17	1	flavorant
17.75	1.28	unknown neryl acetate related compound RRT 1.30	NA	NA	17.7	13.0	13.0	17.5	16.5	15.1	9.1	13.4	16.8	14.7	2.8	9.8E-03	4	demethylated and oxidized neryl acetate
20.68	1.50	(Z)-beta-damascone	23726-92-3	high	27.5	9.0	27.2	28.8	30.7	28.9	29.5	8.8	10.0	22.3	9.8	8.2E-04	1	flavorant

Table S7 LC-HRMS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 3.0% at T=0

RT [min]	RRT	Name	CAS #	Confidence Level	Estimated Amount µg/g									Avg (µg/g)	Stdev	P- Value	Group	Rationalization
					Batch HJ10PG06B			Batch HJ10PH06B			Batch HJ10PI06B							
					Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3					
2.07	0.15	unknown PG_VG related compound RRT 0.16 ^a	NA	NA	11.1	7.1	8.7	9.3	10.8	10.3	9.8	9.7	8.2	9.4	1.3	8.3E- 15	4	dehydration of PG VG to form conjugate
2.41	0.17	hydroxyacetone	116-09- 6	high	13.8	11.3	12.8	13.7	13.5	13.3	14.1	14.8	14.6	13.6	1.0	8.9E- 15	4	dehydration of glycerol and/or oxidation of PG
3.27	0.24	unknown nicotine related compound RRT 0.24	NA	NA	36.0	32.5	31.7	33.7	33.2	33.8	34.4	36.0	33.4	33.9	1.4	5.1E- 02	4	nicotine degradant
4.23	0.31	theobromine	83-67-0	high	3.9	3.2	3.6	3.8	3.7	3.7	4.0	4.2	4.1	3.8	0.3	NA	1	Flavorant
7.22	0.52	caffeine	58-08-2	confirmed	6.4	5.1	5.0	5.9	5.7	5.5	5.9	6.0	5.9	5.7	0.4	1.8E- 04	1	Flavorant
10.25	0.74	2,3-dihydroxypropyl benzoate	3376- 59-8	high	34.7	27.8	28.8	30.0	34.8	31.6	28.9	36.2	35.7	32.0	3.3	1.5E- 14	4	benzoic acid + VG
11.57	0.84	N-methylmyosmine	525-74- 6	high	32.1	28.8	28.7	29.6	30.9	29.9	18.2	33.9	28.8	29.0	4.4	9.0E- 04	4	nicotine degradant
11.78	0.85	1-(1-methyl-5- (pyridin-3-yl)-1H- pyrrol-2-yl)propan-2- one isomer 1	241624 2-88-9	high	6.9	6.9	6.8	8.0	7.6	8.5	6.4	6.8	6.2	7.1	0.8	6.2E- 15	4	nicotine degradant
12.44	0.90	1-(1-methyl-5- (pyridin-3-yl)-1H- pyrrol-2-yl)propan-2- one isomer 2	241624 2-88-9	high	10.5	10.3	11.3	12.6	12.2	14.0	10.5	11.6	10.5	11.5	1.2	9.6E- 16	4	nicotine degradant
13.43	0.97	unknown benzyl alcohol related compound RRT 0.97	NA	NA	16.2	12.9	14.1	15.4	15.0	14.9	15.7	16.4	15.4	15.1	1.1	3.0E- 15	4	methoxylated, oxidized and ring opening of benzyl alcohol
16.27	1.18	2-isopropyl-N, 2, 3- trimethylbutylbutamide	51115- 67-4	high	97.4	78.5	86.9	92.4	88.7	93.1	93.7	97.5	94.5	91.4	6.0	1.5E- 14	1	Flavorant
17.96	1.30	unknown neryl acetate related compound RRT 1.30	NA	NA	48.3	39.9	50.1	52.3	54.5	53.1	55.3	55.7	52.2	51.3	4.9	1.5E- 05	4	demethylated and oxidized neryl acetate
20.69	1.50	(Z)-beta-damascone	23726- 92-3	high	31.7	35.9	25.4	33.3	31.6	31.0	30.5	32.8	7.5	28.8	8.5	5.9E- 02	1	Flavorant

Table S8 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
3.62	Decamethylcyclopentasiloxane Isomer 2	541-02-6	CONFIRMED	4.1	6.7	9.1	8.5	12.2	9.9	10.2	11.5	12.8	9.4	2.8	3	E&L
3.92	Unknown (RRT 0.262)	NA	NA	3.5	3.4	3.6	3.2	3.0	2.7	3.2	3.3	2.7	3.2	0.3	5	NR
4.08	Pyridine	110-86-1	CONFIRMED	0.9	1.0	1.8	1.6	1.2	1.0	0.9	1.6	1.0	1.2	0.3	1	Flavorant
5.04	Hydroxyacetone	116-09-6	CONFIRMED	8.6	9.8	12.6	9.3	8.4	8.4	9.0	12.1	9.6	9.8	1.5	4	dehydration of glycerol and/or oxidation of PG
5.61	1-((ethoxydimethylsilyl)oxy)propan-2-ol	NA	MEDIUM	3.3	3.5	4.0	3.5	3.7	3.5	3.4	3.7	3.6	3.6	0.2	4	hydrolysis of E&L source compound (such as dodecamethylcyclohexasiloxane)
5.94	2-((ethoxydimethylsilyl)oxy)propan-1-ol	NA	MEDIUM	1.7	1.7	2.1	1.8	1.8	1.9	1.6	1.8	1.7	1.8	0.1	4	hydrolysis of E&L source compound (such as dodecamethylcyclohexasiloxane)
6.50	Acetic acid	64-19-7	CONFIRMED	8.6	16.0	12.4	9.8	8.7	10.1	10.7	9.8	9.1	10.6	2.3	1	Flavorant
6.63	Menthone	89-80-5	CONFIRMED	15.5	17.2	17.9	17.7	15.4	16.9	16.6	18.5	16.9	16.9	1.0	4	oxidized menthol
6.70	Menthofuran	494-90-6	CONFIRMED	0.9	0.9	0.9	1.0	0.8	0.9	1.0	1.0	1.0	0.9	0.1	1	Flavorant
6.79	Isomenthone	491-07-6	CONFIRMED	5.8	6.4	6.7	6.6	5.8	6.3	6.1	6.9	6.4	6.3	0.4	1	Flavorant
7.07	1,3Dioxolane-2methanol_2,4dimethyl-Iso1	53951-43-2	MEDIUM	3.0	3.7	3.2	6.5	5.9	6.5	5.8	6.3	6.0	5.2	1.5	4	PG degradant
7.20	1,3Dioxolane-2methanol_2,4dimethyl-Iso2	53951-43-2	MEDIUM	1.3	1.7	1.5	3.3	3.1	3.6	2.8	3.1	2.9	2.6	0.9	4	PG degradant
7.20	Linalool	78-70-6	CONFIRMED	0.9	0.9	0.9	0.9	0.9	0.9	0.9	1.1	0.9	0.9	0.1	1	Flavorant
7.31	Linalyl acetate	115-95-7	CONFIRMED	1.1	1.2	1.3	1.3	1.1	1.2	1.4	1.5	1.3	1.3	0.1	1	Flavorant
7.40	Menthyl acetate	89-48-5	CONFIRMED	3.3	3.8	3.9	3.4	2.9	3.2	3.0	3.4	3.2	3.3	0.3	1	Flavorant
7.42	Isopulegol	89-79-2	CONFIRMED	2.3	2.7	2.7	2.6	2.4	2.5	2.6	2.8	2.6	2.6	0.2	4	reduction of isopulegone
7.50	Unknown Menthol Related Comp.(RRT 0.503)	NA	NA	2.8	2.2	2.4	1.3	1.5	2.0	2.3	2.3	2.3	2.1	0.5	4	Menthol (Flavorant) reaction
7.56	1,3-Dioxolane-4-methanol_2,2-dimethyl-	100-79-8	CONFIRMED	12.1	12.0	10.4	70.1	57.8	75.4	68.2	25.5	23.5	39.5	27.8	4	VG degradant
7.68	Ethanone_1-(2-pyridinyl)-	1122-62-9	CONFIRMED	16.2	18.5	18.2	15.9	13.9	15.7	16.7	18.7	17.0	16.7	1.5	1	Flavorant
7.64	Unknown Siloxane (RRT 0.515)	NA	NA	0.8	1.1	1.1	1.0	0.9	1.1	0.9	1.0	1.0	1.0	0.1	3	E&L
7.78	Terpinen-4-ol	562-74-3	CONFIRMED	0.7	ND	1.0	0.8	ND	0.8	1.0	ND	0.8	0.9	0.1	1	Flavorant

Table S8 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
7.91	Acetylpyrazine	22047-25-2	CONFIRMED	ND	2.3	2.0	2.0	1.8	2.0	1.8	2.0	1.9	2.0	0.2	1	Flavorant
7.97	Unknown Siloxane (RRT 0.532)	NA	NA	ND	ND	0.7	ND	ND	ND	ND	0.8	ND	0.7	0.0	3	E&L
8.00	Methyl benzoate	93-58-3	CONFIRMED	8.7	6.7	12.5	8.1	6.4	5.5	6.2	12.1	7.1	8.1	2.5	4	benzoic acid + MeOH
8.09	Unknown Siloxane (RRT 0.540)	NA	NA	ND	1.6	ND	ND	ND	ND	ND	ND	ND	1.6	0.0	3	E&L
8.12	Unknown Siloxane (RRT 0.542)	NA	NA	0.8	0.8	ND	1.0	1.3	1.1	ND	2.3	0.9	1.2	0.5	3	E&L
8.24	Lavandulol	498-16-8	CONFIRMED	1.7	2.0	1.7	1.8	1.6	1.7	1.7	ND	2.0	1.8	0.2	1	Flavorant
8.20	5-Methyl-2-(1-methylethyl)-Cyclohexanol	1490-04-6	CONFIRMED	3.79	5.02	4.73	4.12	3.86	3.96	4.33	5.05	4.86	4.4	0.5	1	Isomer of menthol (Flavorant)
8.20	Acetophenone	98-86-2	CONFIRMED	ND	ND	1.0	ND	ND	ND	ND	1.1	1.0	1.1	0.1	5	NR
8.21	Pulegone	89-82-7	CONFIRMED	1.8	1.9	2.1	1.9	1.7	1.8	1.9	2.0	1.9	1.9	0.1	1	Flavorant
8.45	Diethoxydimethylsilane	78-62-6	CONFIRMED	16.2	15.0	17.7	17.1	18.6	20.0	16.8	17.5	17.8	17.4	1.4	3	E&L
8.47	1,3-Dioxolane_4-methyl-2-pentyl-	1599-49-1	LOW	2.5	2.7	2.9	7.4	6.4	7.1	6.3	7.0	6.7	5.5	2.1	4	PG + hexanal
8.47	Terpinyl propionate	80-27-3	MEDIUM	ND	0.8	0.8	0.8	ND	0.7	0.8	0.9	0.7	0.8	0.1	1	Flavorant
8.66	Nicotinealdehyde	500-22-1	CONFIRMED	1.5	1.5	1.7	1.5	1.4	1.5	1.5	1.7	1.6	1.5	0.1	4	demethylation of 3-acetylpyridine
8.80	Piperitone	89-81-6	CONFIRMED	ND	0.8	ND	ND	ND	ND	ND	0.7	ND	0.7	0.0	1	Flavorant
9.36	Dipropylene glycol	110-98-5	CONFIRMED	40.9	48.0	45.3	44.7	40.4	43.2	43.7	48.4	44.3	44.3	2.7	4	PG degradant
9.46	Benzaldehyde_2,3-dimethyl-	5779-93-1	MEDIUM	1.0	1.5	1.8	ND	1.1	ND	1.5	1.8	1.5	1.5	0.3	3	E&L
9.50	Benzyl alcohol	100-51-6	CONFIRMED	35.7	43.3	39.9	39.7	35.8	39.3	40.9	44.3	41.2	40.0	2.9	1	Flavorant
9.52	N,2,3-trimethyl-2-isopropylbutamide	51115-67-4	CONFIRMED	68.6	81.3	75.6	73.8	66.3	72.2	73.9	80.2	73.8	74.0	4.8	1	Flavorant
9.61	(Z)-beta-Damascone	23726-92-3*	CONFIRMED	13.1	15.0	15.1	16.0	12.8	13.9	14.7	15.3	14.5	14.5	1.1	1	Flavorant
9.95	2-(4-methoxyphenyl)-1-pyrroline	NA	MEDIUM	4.4	4.1	4.8	4.2	4.6	4.7	4.3	5.4	5.3	4.6	0.5	4	Nicotine degradant
10.11	Unknown Nic.Related Comp.(RRT 0.670)	NA	NA	0.7	1.1	0.9	0.8	0.9	1.3	0.9	1.0	0.9	0.9	0.2	4	Nicotine degradant
10.53	N-methyl-4-(3-pyridyl)-3-buten-1-amine	15585-43-0	HIGH	4.1	5.2	4.7	4.8	4.0	4.6	5.1	5.7	5.1	4.8	0.5	4	Nicotine degradant

Table S8 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
10.55	N-Methylanabasine	24380-92-5	CONFIRMED	2.8	3.1	3.2	3.0	2.9	2.9	3.2	3.6	3.2	3.1	0.2	4	Nicotine degradant
10.55	Phenol	108-95-2	CONFIRMED	2.0	2.1	2.2	1.8	1.9	1.6	1.8	2.3	1.7	1.9	0.2	2	HPHC
11.20	Dihydroxyacetone	96-26-4	CONFIRMED	1.2	1.4	1.4	1.4	1.2	1.1	1.3	1.4	1.0	1.3	0.1	4	oxidation of glycerol
11.58	Unknown Nic.Related Comp.(RRT 0.777)	NA	NA	ND	0.7	ND	ND	ND	ND	0.8	0.8	0.7	0.8	0.1	4	Nicotine degradant
12.30	Piperonal	120-57-0	CONFIRMED	1.7	2.0	1.9	1.7	1.5	1.6	2.5	2.8	2.5	2.0	0.5	1	Flavorant
12.35	Glyceryl monoacetate	106-61-6	CONFIRMED	33.8	43.7	44.9	13.9	13.6	13.2	20.9	25.6	20.8	25.6	12.5	4	VG esterification/transesterification
12.70	3-(1,3-dimethylpyrrol-2-yl)pyridine	78210-38-5	CONFIRMED	4.7	4.8	5.7	4.5	4.4	4.6	4.8	5.6	4.8	4.9	0.5	4	Nicotine degradant
13.57	Unknown Nic. Related Comp.(RRT 0.849)	NA	NA	ND	3.1	2.1	7.8	4.4	4.2	4.0	4.0	3.4	4.1	1.7	4	Nicotine degradant
13.90	3-(1,3-dimethylpyrrol-2-yl)pyridine Iso	78210-38-5	HIGH	1.4	1.4	1.5	1.7	1.6	2.0	2.3	1.9	1.7	1.7	0.3	4	Nicotine degradant
14.31	1,3-Ethoxyethylideneglycerol	NA	MEDIUM	3.2	3.8	4.6	6.9	6.8	7.3	6.5	7.2	6.3	5.9	1.6	4	VG degradant
14.41	Unknown Nic. Related Comp. (RRT 0.956)	NA	NA	ND	ND	ND	ND	ND	1.2	0.8	ND	1.1	1.0	0.2	4	Nicotine degradant
14.53	p-Dioxane-2,5-dimethanol	14236-12-5	CONFIRMED	15.7	18.7	16.7	13.8	12.8	11.9	14.6	16.1	14.8	15.0	2.1	4	2VG dehydration
14.60	Unknown Nic.Related Comp.(RRT 0.970)	NA	NA	3.2	3.4	2.5	6.6	6.4	7.2	5.7	5.7	6.2	5.2	1.7	4	Nicotine degradant
14.66	N-Propylornicotine	91907-45-8	CONFIRMED	2.3	2.6	2.4	2.3	2.0	2.3	3.6	4.0	3.5	2.8	0.7	4	Nicotine degradant
14.70	Bis(2,6-hydroxymethyl) dioxane	54120-69-3	CONFIRMED	63.1	75.5	69.4	49.2	46.2	47.8	54.7	59.1	55.5	57.8	10.0	4	2VG dehydration
14.72	Bis(2,6 hydroxymethyl) dioxane - Iso2	54120-69-3	HIGH	ND	ND	ND	ND	6.3	ND	8.6	ND	ND	7.5	1.7	4	2VG dehydration
14.89	Bis(2,6 hydroxymethyl) dioxane - Iso3	54120-69-3	HIGH	56.2	68.3	59.7	33.0	46.9	29.0	89.9	85.7	67.6	59.6	21.1	4	2VG dehydration
15.00	Bis(2,6-hydroxymethyl) dioxane - Iso4	54120-69-3	HIGH	36.8	44.1	41.4	29.4	27.3	21.6	31.5	34.2	ND	33.3	7.4	4	2VG dehydration
15.19	Unknown Nic.Related Comp.(RRT 1.012)	NA	NA	2.6	ND	5.6	5.3	5.2	4.2	3.2	4.3	4.4	4.4	1.0	4	Nicotine degradant
15.20	Bis(2,6-hydroxymethyl) dioxane - Iso5	54120-69-3	HIGH	13.5	16.0	14.0	13.0	10.8	12.1	12.9	14.6	13.7	13.4	1.5	4	2VG dehydration
15.88	N-Methylnicotinamide	114-33-0	CONFIRMED	0.8	ND	0.7	ND	2.0	ND	ND	ND	ND	1.2	0.7	4	Nicotine degradant
16.80	Hexadecanoic Acid	57-10-3	CONFIRMED	2.3	4.7	2.6	2.1	2.6	2.5	2.2	3.2	2.0	2.7	0.8	3	E&L

Table S8 GC-MS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS#	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
16.84	Unknown (RRT 1.132)	NA	NA	0.9	1.0	1.1	0.9	0.8	1.0	0.9	1.2	0.9	1.0	0.1	5	NR
17.00	2-(beta nicotyrine)acetaldehyde Iso-1 ^a	NA	MEDIUM	1.6	2.6	4.8	2.0	2.3	2.3	1.7	2.1	2.2	2.4	1.0	4	Nicotine degradant
17.50	1-(beta nicotyrine)propan-2-one Iso-1 ^a	2416242-88-9	HIGH	10.7	10.4	10.9	10.4	10.1	10.1	11.1	12.6	11.0	10.8	0.8	4	Nicotine degradant
17.59	Unknown (RRT 1.175)	NA	NA	1.8	ND	2.1	1.6	1.3	1.4	1.5	2.1	ND	1.7	0.0	5	NR
17.70	N-Formylornicotine	3000-81-5	CONFIRMED	ND	0.9	0.7	ND	0.7	ND	ND	ND	0.9	0.8	0.1	4	Nicotine degradant
18.76	Unknown Nic. Related Comp. (RRT 1.246)	NA	NA	1.0	2.0	2.8	1.4	1.1	1.1	0.9	1.0	1.0	1.4	0.6	4	Nicotine degradant
19.08	Caffeine	58-08-2	CONFIRMED	13.0	15.8	14.5	14.7	13.1	14.0	14.0	15.4	14.4	14.3	0.9	1	Flavorant
19.80	1-(beta nicotyrine)propan-2-one Iso-2 ^a	2416242-88-9	HIGH	24.7	24.1	24.9	24.3	22.9	23.1	26.0	28.2	24.7	24.8	1.6	4	Nicotine degradant

^a 1-(beta nicotyrine)propan-2-one: 1-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)propan-2-one

^a 2-(beta nicotyrine)acetaldehyde: 2-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)acetaldehyde

NR = Not Rationalized

Table S9 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
3.62	Decamethylcycl opentasiloxane Isomer 2	541-02-6	CONFIRMED	12.9	10.5	8.7	9.1	7.6	8.9	9.9	11.5	9.4	9.8	1.6	3	E&L
4.08	Pyridine	110-86-1	CONFIRMED	1.4	1.2	1.4	ND	1.2	ND	2.0	1.5	ND	1.4	0.3	1	Flavorant
4.14	1,8-Cineole	470-82-6	HIGH	ND	ND	ND	ND	0.7	ND	0.7	ND	ND	0.7	0.0	1	Flavorant
5.04	Hydroxyacetone	116-09-6	CONFIRMED	8.9	8.7	10.8	9.0	11.1	9.6	10.7	8.3	8.3	9.5	1.1	4	dehydration of glycerol and/or oxidation of PG
5.61	1-((ethoxydimethylsilyl)oxy)propan-2-ol	NA	MEDIUM	ND	ND	ND	ND	ND	ND	ND	0.7	ND	0.7	0.0	4	hydrolysis of E&L source compound (such as dodecamethylcycl hexasiloxane)

Table S9 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
6.50	Acetic acid	64-19-7	CONFIRMED	14.1	9.2	6.2	ND	6.7	8.5	7.4	7.6	ND	8.5	2.6	1	Flavorant
6.63	Menthone	89-80-5	CONFIRMED	16.3	16.5	18.0	16.6	17.1	16.7	19.5	16.4	14.8	16.9	1.3	4	oxidized menthol
6.70	Menthofuran	494-90-6	CONFIRMED	0.8	0.7	0.8	0.7	ND	0.7	0.9	0.7	ND	0.8	0.1	1	Flavorant
6.79	Isomenthone	491-07-6	CONFIRMED	6.3	6.2	6.9	6.3	6.4	6.2	7.4	6.1	5.6	6.4	0.5	1	Flavorant
7.07	1,3Dioxolane-2methanol_2,4dimethyl-Iso1	53951-43-2	MEDIUM	3.4	3.4	3.7	6.5	6.9	6.8	7.1	6.0	5.2	5.4	1.6	4	PG degradant
7.20	1,3Dioxolane-2methanol_2,4dimethyl-Iso2	53951-43-2	MEDIUM	1.6	1.6	1.8	3.1	3.4	3.5	3.6	2.9	2.6	2.7	0.8	4	PG degradant
7.20	Linalool	78-70-6	CONFIRMED	0.9	1.0	1.1	1.0	1.0	0.9	1.2	0.9	0.9	1.0	0.1	1	Flavorant
7.31	Linalyl acetate	115-95-7	CONFIRMED	1.2	1.1	1.2	1.1	1.2	1.2	1.4	1.2	1.1	1.2	0.1	1	Flavorant
7.40	Menthyl acetate	89-48-5	CONFIRMED	3.9	4.1	4.4	3.0	3.1	2.9	3.6	3.0	2.6	3.4	0.6	1	Flavorant
7.42	Isopulegol	89-79-2	CONFIRMED	2.5	2.5	2.9	2.6	2.7	2.6	3.1	2.6	2.2	2.6	0.3	4	reduction of isopulegone
7.56	1,3-Dioxolane-4-methanol_2,2-dimethyl-	100-79-8	CONFIRMED	52.4	58.0	60.9	59.1	56.6	60.2	74.5	44.7	54.7	57.9	8.0	4	VG degradant
7.68	Ethanone_1-(2-pyridinyl)-	1122-62-9	CONFIRMED	17.2	17.2	19.0	15.6	15.6	15.2	19.4	16.3	14.5	16.7	1.7	1	Flavorant
7.78	Terpinen-4-ol	562-74-3	CONFIRMED	0.8	ND	0.9	0.8	0.9	0.8	1.0	0.8	ND	0.9	0.1	1	Flavorant
7.91	Acetylpyrazine	22047-25-2	CONFIRMED	2.0	2.1	2.6	2.0	2.0	1.9	2.3	1.9	1.7	2.0	0.3	1	Flavorant
8.00	Methyl benzoate	93-58-3	CONFIRMED	5.2	4.1	6.2	4.6	4.3	5.7	7.3	4.0	4.1	5.0	1.1	4	benzoic acid + MeOH
8.24	Lavandulol	498-16-8	CONFIRMED	1.8	1.5	1.7	1.1	1.7	1.6	2.0	1.5	1.5	1.6	0.2	1	Flavorant
8.20	5-Methyl-2-(1-methylethyl)-Cyclohexanol	1490-04-6	CONFIRMED	4.1	4.5	3.7	4.0	3.9	4.1	5.3	4.1	3.3	4.1	0.5	1	Isomer of menthol (Flavorant)
8.21	Pulegone	89-82-7	CONFIRMED	1.4	1.4	2.4	2.4	1.4	1.4	1.7	1.4	1.9	1.7	0.4	1	Flavorant

Table S9 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
8.47	1,3-Dioxolane_4-methyl-2-pentyl-	1599-49-1	LOW	ND	ND	ND	7.2	7.3	7.1	7.2	6.3	5.4	6.7	0.7	4	PG + hexanal
8.47	Terpinyl propionate	80-27-3	MEDIUM	0.7	0.9	0.8	0.7	0.7	ND	0.8	0.7	ND	0.8	0.1	1	Flavorant
8.66	Nicotinealdehyde	500-22-1	CONFIRMED	1.5	1.5	1.7	1.4	1.5	1.6	1.6	1.5	1.3	1.5	0.1	4	demethylation of 3-acetylpyridine
8.66	Unknown Nic. Related Comp. (RRT 0.575)	NA	NA	ND	ND	ND	1.5	1.9	ND	1.8	1.6	ND	1.7	0.2	4	Nicotine degradant
8.80	Piperitone	89-81-6	CONFIRMED	ND	ND	0.7	ND	0.7	ND	0.7	0.7	ND	0.7	0.0	1	Flavorant
9.40	beta-Damascenone	23726-93-4	CONFIRMED	3.2	3.3	3.6	3.2	3.3	3.3	4.1	3.4	2.8	3.4	0.3	1	Flavorant
9.52	N,2,3-trimethyl-2-isopropylbutamide	51115-67-4	CONFIRMED	73.4	75.7	81.0	71.7	75.1	73.3	88.3	73.3	63.3	75.0	6.8	1	Flavorant
9.61	(Z)-beta-Damascenone	23726-92-3	CONFIRMED	36.1	33.9	31.4	32.9	33.0	34.3	37.5	32.3	23.6	32.8	3.9	1	Flavorant
9.95	2-(4-methoxyphenyl)-1-pyrroline	NA	MEDIUM	3.4	4.3	3.8	3.8	3.9	4.0	4.5	4.2	3.5	3.9	0.4	4	Nicotine degradant
9.99	Unknown Nic. Related Comp. (RRT 0.663)	NA	NA	3.6	4.0	4.1	3.8	ND	ND	ND	4.1	3.1	3.8	0.4	4	Nicotine degradant
10.11	Unknown Nic. Related Comp. (RRT 0.670)	NA	NA	ND	ND	0.9	ND	0.7	ND	0.9	0.8	ND	0.8	0.1	4	Nicotine degradant
10.53	N-methyl-4-(3-pyridyl)-3-buten-1-amine	15585-43-0	HIGH	4.4	4.8	4.9	4.3	4.7	4.4	6.1	4.9	4.4	4.8	0.6	4	Nicotine degradant
10.55	N-Methylanabasine	24380-92-5	CONFIRMED	2.8	2.9	3.0	2.7	2.8	2.8	3.9	2.9	2.6	2.9	0.4	4	Nicotine degradant
10.55	Phenol	108-95-2	CONFIRMED	ND	ND	1.4	ND	ND	ND	1.7	ND	ND	1.6	0.2	2	HPHC

Table S9 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
10.60	Unknown Nic. Related Comp. (RRT 0.708)	NA	NA	ND	0.8	0.9	0.7	0.7	0.9	ND	ND	ND	0.8	0.1	4	Nicotine degradant
11.10	Unknown Nic. Related Comp. (RRT 0.727)	NA	NA	5.0	4.7	3.2	4.1	2.3	5.4	4.0	4.4	2.8	4.0	1.0	4	Nicotine degradant
11.58	Unknown Nic. Related Comp. (RRT 0.777)	NA	NA	ND	ND	ND	ND	ND	ND	0.9	0.8	ND	0.8	0.1	4	Nicotine degradant
12.30	Piperonal	120-57-0	CONFIRMED	1.8	1.8	2.0	1.6	1.7	1.6	2.9	2.3	2.0	2.0	0.4	1	Flavorant
12.70	Unknown Nic Related Comp. (RRT 0.840)	NA	NA	0.7	ND	ND	ND	ND	ND	ND	ND	ND	0.7	0.0	4	Nicotine degradant
12.70	3-(1,3-dimethylpyrrol-2-yl)pyridine	78210-38-5	CONFIRMED	4.9	4.3	4.9	4.2	4.4	5.1	4.7	4.2	3.8	4.5	0.4	4	Nicotine degradant
12.76	Propanedioic acid	141-82-2	LOW	29.8	31.7	33.3	ND	ND	ND	ND	ND	ND	31.6	1.7	4	propionic acid to hydroxypropionic acid, followed by oxidation
12.89	Unknown Nic. Related Comp. (RRT 0.855)	NA	NA	4.2	4.9	5.7	7.3	7.8	7.6	8.8	7.0	5.6	6.6	1.5	4	Nicotine degradant
13.57	Unknown Nic. Related Comp. (RRT 0.849)	NA	NA	ND	2.9	ND	3.5	4.1	4.4	4.7	3.8	3.2	3.8	0.7	4	Nicotine degradant
13.90	3-(1,3-dimethylpyrrol-2-yl)pyridine Iso	78210-38-5	HIGH	3.5	3.2	3.6	3.3	3.3	4.3	4.3	3.6	3.3	3.6	0.4	4	Nicotine degradant
13.99	2-hydroxypropyl benzoate	37086-84-3	CONFIRMED	11.0	11.3	12.6	12.6	13.5	13.6	16.1	13.5	11.8	12.9	1.5	4	benzoic acid with alcohol esterification
14.31	1,3-Ethoxyethylidene glycerol	NA	MEDIUM	2.6	2.5	ND	5.5	5.3	5.8	6.2	5.0	4.2	4.6	1.4	4	VG degradant
14.53	p-Dioxane-2,5-dimethanol	14236-12-5	CONFIRMED	17.7	18.6	17.3	12.7	13.4	13.1	17.0	14.1	12.4	15.1	2.4	4	2VG dehydration
14.60	Unknown Nic. Related	NA	NA	2.5	3.4	4.0	5.5	5.2	5.6	5.8	4.7	4.6	4.6	1.1	4	Nicotine degradant

Table S9 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
	Comp.(RRT 0.970)															
14.66	N-Propyl nicotinic acid	91907-45-8	CONFIRMED	2.8	2.9	3.0	2.6	2.6	2.9	4.7	3.9	3.2	3.2	0.7	4	Nicotine degradant
14.70	Bis(2,6-hydroxymethyl) dioxane	54120-69-3	CONFIRMED	63.0	46.6	45.9	31.3	31.5	32.3	63.2	51.0	45.2	45.6	12.4	4	2VG dehydration
14.89	Bis(2,6-hydroxymethyl) dioxane - Iso3	54120-69-3	HIGH	30.3	31.7	33.9	21.9	22.5	23.0	29.9	23.3	156.3	41.4	43.3	4	2VG dehydration
15.00	Bis(2,6-hydroxymethyl) dioxane - Iso4	54120-69-3	HIGH	36.1	40.5	39.1	25.7	28.0	26.8	42.1	29.9	27.0	32.8	6.6	4	2VG dehydration
15.19	Unknown Nic.Related Comp.(RRT 1.012)	NA	NA	2.1	1.3	ND	4.3	4.0	4.1	4.5	3.3	3.3	3.3	1.1	4	Nicotine degradant
15.20	Bis(2,6-hydroxymethyl) dioxane - Iso5	54120-69-3	HIGH	12.2	18.5	13.4	10.0	10.7	10.0	13.7	11.1	9.8	12.1	2.8	4	2VG dehydration
16.50	Unknown Nic. Related Comp. (RRT 1.098)	NA	NA	2.0	1.9	3.5	ND	2.0	1.4	2.0	1.8	ND	2.1	0.6	4	Nicotine degradant
16.56	Unknown (RRT 1.098)	NA	NA	ND	ND	ND	ND	ND	ND	ND	ND	1.3	1.3	0.0	5	NR
16.80	Hexadecanoic Acid	57-10-3	CONFIRMED	6.0	3.8	2.6	3.0	2.9	3.3	4.2	3.2	1.8	3.4	1.2	3	E&L
17.00	2-(beta nicotyrine)acetaldehyde Iso-1 ^a	NA	MEDIUM	0.9	ND	1.6	0.8	7.4	0.7	1.2	ND	2.9	2.2	2.4	4	Nicotine degradant
17.36	Phenol_2-(1-phenylethyl)-	4237-44-9	CONFIRMED	1.0	1.4	ND	ND	0.9	ND	ND	ND	ND	1.1	0.3	4	Phenylethanol (from phenylethyl acetate) + phenol
17.50	1-(beta nicotyrine)propan-2-one Iso-1 ^a	2416242-88-9	HIGH	9.1	8.8	9.9	8.6	9.0	12.1	10.7	9.3	9.0	9.6	1.1	4	Nicotine degradant
18.60	Octadecanoic acid	57-11-4	CONFIRMED	ND	2.0	2.1	2.5	ND	2.6	1.0	ND	ND	2.0	0.6	3	E&L
18.76	Unknown Nic. Related Comp. (RRT 1.246)	NA	NA	2.0	1.7	3.4	2.0	6.4	1.2	1.8	3.6	2.2	2.7	1.6	4	Nicotine degradant

Table S9 GC-MS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

Library Retention Time (min)	Compound	CAS #	Identification Confidence	Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A			Avg (µg/g)	Stdev	Group	Rationalization
				Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)	Rep-1 (µg/g)	Rep-2 (µg/g)	Rep-3 (µg/g)				
19.08	Caffeine	58-08-2	CONFIRMED	12.9	14.4	14.1	13.1	14.0	13.6	16.2	12.8	11.7	13.6	1.3	1	Flavorant
19.80	1-(beta nicotyrine)propan-2-one Iso-2 ^a	2416242-88-9	HIGH	21.0	21.3	24.0	21.4	21.7	26.0	25.7	22.4	21.6	22.8	2.0	4	Nicotine degradant

^a 1-(beta nicotyrine)propan-2-one: 1-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)propan-2-one

^a 2-(beta nicotyrine)acetaldehyde: 2-(1-methyl-5-(pyridine-3-yl)-1H-pyrrol-2-yl)acetaldehyde

NR = Not Rationalized

Table S10 LC-HRMS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

RT [min]	RRT	Name	CAS #	Confidence Level	Estimated Amount µg/g									Avg (µg/g)	Stddev	P-Value	Group	Rationalization
					Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A							
					Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3					
2.14	0.16	unknown PG_VG related compound RRT 0.16	NA	NA	3.6	3.1	5	3.6	4.1	3.5	4.2	3	3.7	3.8	0.6	4.70E-09	4	dehydration of PG VG to form conjugate
2.25	0.17	unknown PG_VG related compound RRT 0.17	NA	NA	31.4	27.5	30.4	31.4	37	29.7	32	37	36.6	32.6	3.5	3.60E-10	4	dehydration of PG VG to form conjugate
2.44	0.18	Hydroxyacetone	116-09-6	high	5.7	4.2	5	3.6	5.3	3.6	4.5	4.1	4.4	4.5	0.7	4.40E-03	4	dehydration of glycerol and/or oxidation of PG
2.63	0.19	4- methoxybenzaldehyde	123-11-5	high	4.2	3	3.5	3.2	3.8	3.1	3.9	3.8	3.6	3.6	0.4	3.00E-02	4	methoxylated benzaldehyde
3.09	0.23	unknown nicotine related compound RRT 0.23	NA	NA	30.4	29.4	28.2	39.3	25.1	39.9	26.8	22.9	36.1	30.9	6.2	4.50E-05	4	nicotine degradant
4.23	0.31	theobromine	83-67-0	high	6.5	4.9	5.1	5.2	6.4	4.2	6.2	6.1	6.4	5.7	0.8	1.00E-10	1	Flavorant
6.99	0.51	caffeine	58-08-2	confirmed	19.6	17.4	22.6	32.1	19.1	23.2	17.2	19.4	19.6	21.1	4.6	NA	1	Flavorant
9.69	0.71	unknown nicotine related compound RRT 0.71	NA	NA	6.9	6.9	8.8	10.6	8.8	9	7.4	7.9	7.5	8.2	1.2	7.30E-03	4	nicotine degradant
10	0.74	2,3-dihydroxypropyl benzoate	3376-59-8	high	75.8	61.9	61.9	58.4	107.6	61.6	82.1	79.7	84.5	74.8	15.9	1.40E-09	4	benzoic acid + VG

Table S10 LC-HRMS Characterization of Aerosol Collected Under Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

RT [min]	RRT	Name	CAS #	Confidence Level	Estimated Amount µg/g									Avg (µg/g)	Stdev	P-Value	Group	Rationalization
					Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A							
					Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3					
11.28	0.83	N-methylmyosmine	525-74-6	high	17.7	14.4	14.3	18	19.4	17.5	20	15.4	20.2	17.4	2.3	3.00E-05	4	nicotine degradant
11.57	0.85	1-(1-methyl-5-(pyridin-3-yl)propan-2-one isomer 1	2416242-88-9	high	9.1	7	7.2	7.1	9.5	6.4	8.1	9.8	5.8	7.8	1.4	NA	4	nicotine degradant
12.24	0.9	1-(1-methyl-5-(pyridin-3-yl)propan-2-one isomer 2	2416242-88-9	high	17.5	13.6	13.2	13.8	12.1	12.6	14.5	15.4	15.3	14.2	1.7	1.10E-09	4	nicotine degradant
13.16	0.97	unknown benzyl alcohol related compound RRT 0.97	NA	NA	42.2	29.5	36.5	34.9	43.6	32.8	39.3	39.7	44	38.1	5	2.80E-09	4	methoxylated, oxidized and ring opening of benzyl alcohol
16.24	1.2	2-isopropyl-N, 2, 3-trimethylbutylbutamide	51115-67-4	high	79.8	102	87.9	93.7	80.7	90.6	88.3	92.6	91.8	89.7	6.8	NA	1	flavorant
17.71	1.3	unknown neryl acetate related compound RRT 1.30	NA	NA	64	39.9	45.3	54.8	61.8	47	62.1	69.2	69.4	57.1	10.8	1.20E-08	4	demethylated and oxidized neryl acetate
20.45	1.51	(Z)-beta-damascone	23726-92-3	high	10.2	7.3	13	13.8	19.7	10.1	10.3	9	15.5	12.1	3.8	4.10E-07	1	flavorant

Table S11 LC-HRMS Characterization of Aerosol Collected Under Non-Intense Puffing Regime from Three Batches of Menthol 5.0% at T=0

RT [min]	RRT	Name	CAS #	Confidence Level	Estimated Amount µg/g									Avg (µg/g)	Stdev	P- Value	Group	Rationalization
					Batch HH26PG06A			Batch HH26PH06A			Batch HH26PI06A							
					Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3	Rep 1	Rep 2	Rep 3					
2.14	0.16	unknown PG_VG related compound RRT 0.16	NA	NA	4.1	6.6	3.4	5.2	4.8	3.0	2.7	2.6	5.0	4.2	1.4	NA	4	dehydration of PG VG to form conjugate
2.25	0.17	unknown PG_VG related compound RRT 0.17	NA	NA	26.3	32.2	29.7	32.1	33.1	30.1	29.0	36.5	39.8	32.1	4.1	2.00E- 04	4	dehydration of PG VG to form conjugate
2.44	0.18	Hydroxyacetone	116-09-6	high	3.6	4.9	5.2	3.5	3.7	3.5	2.8	3.5	4.0	3.8	0.8	7.40E- 03	4	dehydration of glycerol and/or oxidation of PG
3.06	0.23	unknown nicotine related compound RRT 0.23	NA	NA	23.5	22.4	19.2	24.5	27.2	17.7	20.3	30.6	29.3	23.9	4.5	1.00E- 02	4	nicotine degradant
4.23	0.31	theobromine	83-67-0	high	5.3	6.1	6.3	5.5	5.8	5.0	5.0	6.2	6.6	5.7	0.6	8.50E- 15	1	Flavorant
6.98	0.51	caffeine	58-08-2	confirmed	14.8	20.3	15.8	22.4	24.2	28.9	15.6	24.1	18.1	20.5	4.8	NA	1	Flavorant
10.00	0.74	2,3-dihydroxypropyl benzoate	3376-59- 8	high	51.0	57.3	75.9	62.7	59.6	54.1	57.2	63.7	73.8	61.7	8.4	1.30E- 05	4	benzoic acid + VG
11.18	0.82	N-methylmyosmine	525-74-6	high	13.1	13.1	15.7	16.5	19.3	12.1	14.1	16.5	18.0	15.4	2.4	5.70E- 04	4	nicotine degradant
11.58	0.85	1-(1-methyl-5- (pyridin-3-yl)propan-2- one isomer 1	2416242- 88-9	high	6.3	7.0	8.7	6.2	7.0	7.6	5.6	7.4	7.6	7.0	0.9	7.80E- 11	4	nicotine degradant
12.23	0.90	1-(1-methyl-5- (pyridin-3-yl)propan-2- one isomer 2	2416242- 88-9	high	12.2	13.5	15.6	12.0	14.8	9.4	11.3	14.2	11.8	12.7	1.9	3.40E- 12	4	nicotine degradant
13.16	0.97	unknown benzyl alcohol related compound RRT 0.97	NA	NA	32.3	38.0	36.0	34.5	37.2	31.2	35.0	40.4	41.4	36.2	3.4	2.40E- 04	4	methoxylated, oxidized and ring opening of benzyl alcohol
13.26	0.98	2-isopropyl-N, 2, 3- trimethylbutylbutamide	51115- 67-4	high	80.0	83.8	80.1	87.7	81.5	82.1	90.2	81.8	70.3	81.9	5.6	NA	1	Flavorant
17.70	1.30	unknown neryl acetate related compound RRT 1.30	NA	NA	34.5	40.5	56.2	46.8	39.1	34.4	46.3	63.1	69.9	47.9	12.6	1.30E- 08	4	demethylated and oxidized neryl acetate
20.41	1.50	(Z)-beta-damascone	23726- 92-3	high	6.1	11.6	11.8	11.9	13.9	14.6	10.7	11.0	15.4	11.9	2.7	NA	1	Flavorant

Table S12 List of Compounds Detected in The Aerosol Collected from JUUL Menthol 3.0% at the Initial Timepoint (T=0) Under Intense and Non-Intense Puffing Regimes by Non-Targeted Analyses

Chemical	CAS#	Potential Source	Smoke/Aerosol	Average (ug/g)	Group
(Z)-beta-damascone	23726-92-3	Flavorant	Smoke	16.7	1
1-((ethoxydimethylsilyl)oxy)propan-2-ol	NA	hydrolysis of E&L source compound (such as dodecamethylcyclohexasiloxane)	Aerosol	1	4
1-(beta nicotyrine)propan-2-one Iso-1	2416242-88-9	Nicotine degradant	Aerosol	6.2	4
1-(beta nicotyrine)propan-2-one Iso-2	2416242-88-9	Nicotine degradant	Aerosol	14	4
1,3-Dioxolane_4-methyl-2-pentyl-	1599-49-1	PG + hexanal	Aerosol	2.5	4
1,3Dioxolane-2methanol_2,4dimethyl-Iso1	53951-43-2	PG degradant	Aerosol	2.6	4
1,3Dioxolane-2methanol_2,4dimethyl-Iso2	53951-43-2	PG degradant	Aerosol	1.4	4
1,3-Dioxolane-4-methanol_2,2-dimethyl-	100-79-8	VG degradant	Smoke	35.5	4
1,3-Ethoxyethylideneglycerol	NA	VG degradant	Aerosol	4.1	4
1,8-Cineole	470-82-6	Flavorant	Smoke	0.8	1
2-(4-methoxyphenyl)1-pyrroline	NA	Nicotine degradant	Aerosol	2.6	4
2-(4-methoxyphenyl)-1-pyrroline	NA	Nicotine degradant	Aerosol	3.5	4
2-(beta nicotyrine)acetaldehyde Iso-1	NA	Nicotine degradant	Aerosol	1.2	4
2-(beta nicotyrine)acetaldehyde Iso-2	NA	Nicotine degradant	Aerosol	1.5	4
2,3-dihydroxypropyl benzoate	3376-59-8	benzoic acid + VG	Aerosol	40.2	4
2-ethyl-1-hexanol	104-76-7	E&L	Smoke	0.9	3
2-hydroxypropyl benzoate	37086-84-3	benzoic acid + PG (esterification)	Aerosol	7.2	4
3-(1,3-dimethylpyrrol-2-yl)pyridine	78210-38-5	Nicotine degradant	Smoke	2.6	4
3-(1,3-dimethylpyrrol-2-yl)pyridine Iso	78210-38-5	Nicotine degradant	Smoke	2	4
4-methoxybenzaldehyde	123-11-5	methoxylated benzaldehyde	Smoke	4	4
5-Methyl-2-(1-methylethyl)-Cyclohexanol	1490-04-6	Isomer of menthol (Flavorant)	Smoke	4.4	1
Acetic acid	64-19-7	Flavorant	Smoke	11.3	1
Acetylpyrazine	22047-25-2	Flavorant	Smoke	2.2	1
Benzaldehyde_2,3-dimethyl-	5779-93-1	E&L	Aerosol	1.4	3

Benzyl alcohol	100-51-6	Flavorant	Smoke	37.7	1
beta-Damascenone	23726-93-4	Flavorant	Smoke	3.7	1
Bis(2,6-hydroxymethyl) dioxane	54120-69-3	2VG dehydration	Aerosol	49.9	4
Bis(2,6-hydroxymethyl) dioxane - Iso2	54120-69-3	2VG dehydration	Aerosol	38.2	4
Bis(2,6-hydroxymethyl) dioxane - Iso3	54120-69-3	2VG dehydration	Aerosol	55.5	4
Bis(2,6-hydroxymethyl) dioxane - Iso4	54120-69-3	2VG dehydration	Aerosol	28.4	4
Bis(2,6-hydroxymethyl) dioxane - Iso5	54120-69-3	2VG dehydration	Aerosol	11.5	4
Borneol	464-45-9	α -pinene protonation, capture of this carbocation by H2O accompanied by rearrangement of bicyclo carbon skeleton	Smoke	0.7	4
Caffeine	58-08-2	Flavorant	Smoke	14.2	1
Decamethylcyclopentasiloxane Isomer 3	541-02-6	E&L	Aerosol	12.6	3
Diethoxydimethylsilane	78-62-6	E&L	Aerosol	4.3	3
Dihydroxyacetone	96-26-4	Oxidation of glycerol	Smoke	1.2	4
Dipropylene glycol	110-98-5	2PG - H2O	Smoke	42.7	4
Dodecamethylcyclohexasiloxane Isomer 1	540-97-6	E&L	Aerosol	20.8	3
Ethanone_1-(2-pyridinyl)-	1122-62-9	Flavorant	Smoke	17.8	1
Glyceryl monoacetate	106-61-6	VG esterification/transesterification	Smoke	14.4	4
Hexadecamethylcyclooctasiloxane	556-68-3	E&L	Aerosol	1.9	3
Hexadecanoic Acid	57-10-3	E&L	Smoke	11.5	3
Hydroxyacetone	116-09-6	dehydration of glycerol and/or oxidation of PG	Smoke	9.9	4
Isomenthone	491-07-6	Flavorant	Aerosol	6.8	1
Isopulegol Isomer	7786-67-6	reduction of isopulegone	Aerosol	0.8	4
Lavandulol	498-16-8	Flavorant	Aerosol	2.5	1
Linalool	78-70-6	Flavorant	Smoke	1	1
Linalyl acetate	115-95-7	Flavorant	Aerosol	1.5	1
Menthofuran	494-90-6	Flavorant	Smoke	1.3	1
Menthone	89-80-5	oxidized menthol	Smoke	22	4

Menthyl acetate	89-48-5	Flavorant	Aerosol	3.6	1
Methyl benzoate	93-58-3	benzoic acid + MeOH	Smoke	3.8	4
N,2,3-trimethyl-2-isopropylbutamide	51115-67-4	Flavorant	Aerosol	81.2	1
Nicotinealdehyde	500-22-1	demethylation of 3-acetylpyridine	Smoke	1	4
N-methyl-4-(3-pyridyl)-3-buten-1-amine	15585-43-0	Nicotine degradant	Aerosol	2.5	4
N-Methylanabasine	24380-92-5	Nicotine degradant	Smoke	1.8	4
N-methylmyosmine	525-74-6	nicotine degradant	Smoke	29	4
N-Propylornicotine	91907-45-8	Nicotine degradant	Aerosol	1.6	4
Octadecamethyl-cyclononasiloxane	556-71-8	E&L	Aerosol	0.8	3
p-Dioxane-2,5-dimethanol	14236-12-5	2VG dehydration	Aerosol	13.5	4
Phenol	108-95-2	HPHC	Smoke	1.3	2
Phenol_2-(1-phenylethyl)-	4237-44-9	Phenylethanol (from phenylethyl acetate) + phenol	Aerosol	1.4	4
Piperitone	89-81-6	Flavorant	Smoke	0.8	1
Piperonal	120-57-0	Flavorant	Smoke	2.6	1
Pulegone	89-82-7	Flavorant	Aerosol	2.7	1
Pyridine	110-86-1	Flavorant	Smoke	1.2	1
Terpinen-4-ol	562-74-3	Flavorant	Smoke	1.1	1
Terpinyl propionate	80-27-3	Flavorant	Aerosol	1.1	1
Tetradecamethylcycloheptasiloxane	107-50-6	E&L	Aerosol	8.7	3
theobromine	83-67-0	Flavorant	Smoke	3.8	1
Triacetin	102-76-1	acetic acid + glycerol	Smoke	1.6	4
Unknown (RRT 0.559)	NA	NR	Aerosol	0.9	5
Unknown (RRT 0.724)	NA	NR	Aerosol	3.7	5
unknown benzyl alcohol related compound RRT 0.97	NA	methoxylated, oxidized and ring opening of benzyl alcohol	Aerosol	15.1	4
Unknown Long Chain Alkane (RRT 1.482)	NA	NR	Aerosol	17	5
Unknown Menthol Related Comp (RRT 0.520)	NA	Menthol (Flavorant) reaction	Aerosol	5.6	4
Unknown Menthol Related Comp.(RRT 0.503)	NA	Menthol (Flavorant) reaction	Aerosol	1.9	4

Unknown Menthol Related Comp.(RRT 0.523)	NA	Menthol (Flavorant) reaction	Aerosol	0.9	4
unknown neryl acetate related compound RRT 1.30	NA	demethylated and oxidized neryl acetate	Aerosol	51.3	4
Unknown Nic Related Comp.(RRT 0.743)	NA	Nicotine degradant	Aerosol	1.2	4
Unknown Nic. Related Comp. (RRT 1.098)	NA	Nicotine degradant	Aerosol	1.8	4
Unknown Nic. Related Comp.(RRT 0.849)	NA	Nicotine degradant	Aerosol	4.1	4
Unknown Nic.Related Comp.(RRT 0.840)	NA	Nicotine degradant	Aerosol	3.2	4
Unknown Nic.Related Comp.(RRT 0.923)A	NA	Nicotine degradant	Aerosol	1.3	4
Unknown Nic.Related Comp.(RRT 0.956)	NA	Nicotine degradant	Aerosol	1.5	4
Unknown Nic.Related Comp.(RRT 0.970)	NA	Nicotine degradant	Aerosol	4.4	4
Unknown Nic.Related Comp.(RRT 1.012)	NA	Nicotine degradant	Aerosol	4.3	4
unknown nicotine related compound RRT 0.24	NA	nicotine degradant	Aerosol	36.3	4
unknown PG_VG related compound RRT 0.16a	NA	dehydration of PG VG to form conjugate	Aerosol	9.4	4

Table S13 List of Compounds Detected in The Aerosol Collected from JUUL Menthol 5.0% at the Initial Timepoint (T=0) Under Intense and Non-Intense Puffing Regimes by Non-Targeted Analyses

Chemical	CAS#	Potential Source	Smoke/Aerosol	Average (ug/g)	Group
(Z)-beta-Damascone	23726-92-3	Flavorant	Smoke	32.8	1
1-((ethoxydimethylsilyl)oxy)propan-2-ol	NA	hydrolysis of E&L source compound (such as dodecamethylcyclohexasiloxane)	Aerosol	3.6	4
1-(beta nicotyrine)propan-2-one Iso-1	2416242-88-9	Nicotine degradant	Aerosol	10.8	4
1-(beta nicotyrine)propan-2-one Iso-2	2416242-88-9	Nicotine degradant	Aerosol	24.8	4
1,3-Dioxolane_4-methyl-2-pentyl-	1599-49-1	PG + hexanal	Aerosol	6.7	4
1,3Dioxolane-2methanol_2,4dimethyl-Iso1	53951-43-2	PG degradant	Aerosol	5.4	4
1,3Dioxolane-2methanol_2,4dimethyl-Iso2	53951-43-2	PG degradant	Aerosol	2.7	4
1,3-Dioxolane-4-methanol_2,2-dimethyl-	100-79-8	VG degradant	Smoke	57.9	4
1,3-Ethoxyethylideneglycerol	NA	VG degradant	Aerosol	5.9	4
1,8-Cineole	470-82-6	Flavorant	Smoke	0.7	1
2-((ethoxydimethylsilyl)oxy)propan-1-ol	NA	hydrolysis of E&L source compound (such as dodecamethylcyclohexasiloxane)	Aerosol	1.8	4
2-(4-methoxyphenyl)-1-pyrroline	NA	Nicotine degradant	Aerosol	4.6	4
2-(beta nicotyrine)acetaldehyde Iso-1	NA	Nicotine degradant	Aerosol	2.4	4
2,3-dihydroxypropyl benzoate	3376-59-8	benzoic acid + VG	Aerosol	74.8	4
2-hydroxypropyl benzoate	37086-84-3	benzoic acid with alcohol esterification	Aerosol	12.9	4
3-(1,3-dimethylpyrrol-2-yl)pyridine	78210-38-5	Nicotine degradant	Smoke	4.9	4
3-(1,3-dimethylpyrrol-2-yl)pyridine Iso	78210-38-5	Nicotine degradant	Smoke	3.6	4
4-methoxybenzaldehyde	123-11-5	methoxylated benzaldehyde	Smoke	3.6	4
5-Methyl-2-(1-methylethyl)-Cyclohexanol	1490-04-6	Isomer of menthol (Flavorant)	Smoke	4.4	1
Acetic acid	64-19-7	Flavorant	Smoke	10.6	1
Acetophenone	98-86-2	NR	Smoke	1.1	5
Acetylpyrazine	22047-25-2	Flavorant	Smoke	2	1
Benzaldehyde_2,3-dimethyl-	5779-93-1	E&L	Aerosol	1.5	3
Benzyl alcohol	100-51-6	Flavorant	Smoke	40	1

beta-Damascenone	23726-93-4	Flavorant	Smoke	3.4	1
Bis(2,6 hydroxymethyl) dioxane - Iso3	54120-69-3	2VG dehydration	Aerosol	59.6	4
Bis(2,6-hydroxymethyl) dioxane	54120-69-3	2VG dehydration	Aerosol	57.8	4
Bis(2,6-hydroxymethyl) dioxane - Iso2	54120-69-3	2VG dehydration	Aerosol	7.5	4
Bis(2,6-hydroxymethyl) dioxane - Iso4	54120-69-3	2VG dehydration	Aerosol	33.3	4
Bis(2,6-hydroxymethyl) dioxane - Iso5	54120-69-3	2VG dehydration	Aerosol	13.4	4
Caffeine	58-08-2	Flavorant	Smoke	14.3	1
Decamethylcyclopentasiloxane Isomer 2	541-02-6	E&L	Aerosol	9.8	3
Diethoxydimethylsilane	78-62-6	E&L	Aerosol	17.4	3
Dihydroxyacetone	96-26-4	oxidation of glycerol	Smoke	1.3	4
Dipropylene glycol	110-98-5	PG degradant	Smoke	44.3	4
Ethanone_1-(2-pyridinyl)-	1122-62-9	Flavorant	Smoke	16.7	1
Glyceryl monoacetate	106-61-6	VG esterification/transesterification	Smoke	25.6	4
Hexadecanoic Acid	57-10-3	E&L	Smoke	3.4	3
Hydroxyacetone	116-09-6	dehydration of glycerol and/or oxidation of PG	Smoke	9.8	4
Isomenthone	491-07-6	Flavorant	Aerosol	6.4	1
Isopulegol	89-79-2	reduction of isopulegone	Aerosol	2.6	4
Lavandulol	498-16-8	Flavorant	Aerosol	1.8	1
Linalool	78-70-6	Flavorant	Smoke	1	1
Linalyl acetate	115-95-7	Flavorant	Aerosol	1.3	1
Menthofuran	494-90-6	Flavorant	Smoke	0.9	1
Menthone	89-80-5	oxidized menthol	Smoke	16.9	4
Menthyl acetate	89-48-5	Flavorant	Aerosol	3.4	1
Methyl benzoate	93-58-3	benzoic acid + MeOH	Smoke	8.1	4
N,2,3-trimethyl-2-isopropylbutamide	51115-67-4	Flavorant	Aerosol	75	1
N-Formylnormicotine	3000-81-5	Nicotine degradant	Smoke	0.8	4
Nicotinaldehyde	500-22-1	demethylation of 3-acetylpyridine	Smoke	1.5	4
N-methyl-4-(3-pyridyl)-3-buten-1-amine	15585-43-0	Nicotine degradant	Aerosol	4.8	4
N-Methylanabasine	24380-92-5	Nicotine degradant	Smoke	3.1	4
N-methylmyosmine	525-74-6	nicotine degradant	Smoke	17.4	4

N-Methylnicotinamide	114-33-0	Nicotine degradant	Smoke	1.2	4
N-Propylnornicotine	91907-45-8	Nicotine degradant	Aerosol	3.2	4
Octadecanoic acid	57-11-4	E&L	Smoke	2	3
p-Dioxane-2,5-dimethanol	14236-12-5	2VG dehydration	Aerosol	15.1	4
Phenol	108-95-2	HPHC	Smoke	1.9	2
Phenol_2-(1-phenylethyl)-	4237-44-9	Phenylethanol (from phenylethyl acetate) + phenol	Aerosol	1.1	4
Piperitone	89-81-6	Flavorant	Smoke	0.7	1
Piperonal	120-57-0	Flavorant	Smoke	2	1
Propanedioic acid	141-82-2	propionic acid to hydroxypropionic acid, followed by oxidation	Smoke	31.6	4
Pulegone	89-82-7	Flavorant	Aerosol	1.9	1
Pyridine	110-86-1	Flavorant	Smoke	1.4	1
Terpinen-4-ol	562-74-3	Flavorant	Smoke	0.9	1
Terpinyl propionate	80-27-3	Flavorant	Aerosol	0.8	1
theobromine	83-67-0	Flavorant	Smoke	5.7	1
Unknown (RRT 0.262)	NA	NR	Aerosol	3.2	5
Unknown (RRT 1.098)	NA	NR	Aerosol	1.3	5
Unknown (RRT 1.132)	NA	NR	Aerosol	1	5
Unknown (RRT 1.175)	NA	NR	Aerosol	1.7	5
unknown benzyl alcohol related compound RRT 0.97	NA	methoxylated, oxidized and ring opening of benzyl alcohol	Aerosol	38.1	4
Unknown Menthol Related Comp.(RRT 0.503)	NA	Menthol (Flavorant) reaction	Aerosol	2.1	4
unknown neryl acetate related compound RRT 1.30	NA	demethylated and oxidized neryl acetate	Aerosol	57.1	4
Unknown Nic. Related Comp. (RRT 0.575)	NA	Nicotine degradant	Aerosol	1.7	4
Unknown Nic. Related Comp. (RRT 0.663)	NA	Nicotine degradant	Aerosol	3.8	4
Unknown Nic. Related Comp. (RRT 0.670)	NA	Nicotine degradant	Aerosol	0.9	4
Unknown Nic. Related Comp. (RRT 0.708)	NA	Nicotine degradant	Aerosol	0.8	4
Unknown Nic. Related Comp. (RRT 0.727)	NA	Nicotine degradant	Aerosol	4	4
Unknown Nic. Related Comp. (RRT 0.777)	NA	Nicotine degradant	Aerosol	0.8	4
Unknown Nic. Related Comp. (RRT 0.840)	NA	Nicotine degradant	Aerosol	0.7	4
Unknown Nic. Related Comp. (RRT 0.849)	NA	Nicotine degradant	Aerosol	4.1	4
Unknown Nic. Related Comp. (RRT 0.855)	NA	Nicotine degradant	Aerosol	6.6	4

Unknown Nic. Related Comp. (RRT 0.956)	NA	Nicotine degradant	Aerosol	1	4
Unknown Nic. Related Comp. (RRT 0.970)	NA	Nicotine degradant	Aerosol	5.2	4
Unknown Nic. Related Comp. (RRT 1.012)	NA	Nicotine degradant	Aerosol	4.4	4
Unknown Nic. Related Comp. (RRT 1.098)	NA	Nicotine degradant	Aerosol	2.1	4
Unknown Nic. Related Comp. (RRT 1.246)	NA	Nicotine degradant	Aerosol	2.7	4
unknown nicotine related compound RRT 0.23	NA	nicotine degradant	Aerosol	30.9	4
unknown nicotine related compound RRT 0.71	NA	nicotine degradant	Aerosol	8.2	4
unknown PG_VG related compound RRT 0.16	NA	dehydration of PG VG to form conjugate	Aerosol	4.2	4
unknown PG_VG related compound RRT 0.17	NA	dehydration of PG VG to form conjugate	Aerosol	32.6	4
Unknown Siloxane (RRT 0.515)	NA	E&L	Aerosol	1	3
Unknown Siloxane (RRT 0.532)	NA	E&L	Aerosol	0.7	3
Unknown Siloxane (RRT 0.540)	NA	E&L	Aerosol	1.6	3
Unknown Siloxane (RRT 0.542)	NA	E&L	Aerosol	1.2	3

Table S14. Confidence Levels of Compounds Identified by LC–HRMS NTA.

Confirmed	Comparison to standard reference material
High	High mass accuracy measurement generated a molecular formula which was consistent with a rationalized identification
Medium	Automated search of a library with MS/MS spectral peaks in common
Low	Manual search of online library for best spectral match
NA	Not applicable

Table S15. Confidence Levels of Compounds Identified by GC–MS NTA.

Confirmed	Identification confirmed by comparison to standard reference material by high and unit mass resolution mass spectrometry
High	A mass spectrum match factor score of 850 to 1000
Medium	A mass spectrum match factor score of 700 to 849
Low	A mass spectrum match factor score of 500 to 699
NA	Not Applicable