Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary Information

Particulate Metals and Organic Compounds from Electronic and Tobacco-containing Cigarettes: Comparison of Emission Rates and Secondhand Exposure

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Figure S1. Average total mass concentration of indoor PM (µg/m^3) corresponding to e-cigarette samples without nicotine and e-cigarette samples with nicotine. Error bars represent one standard error.

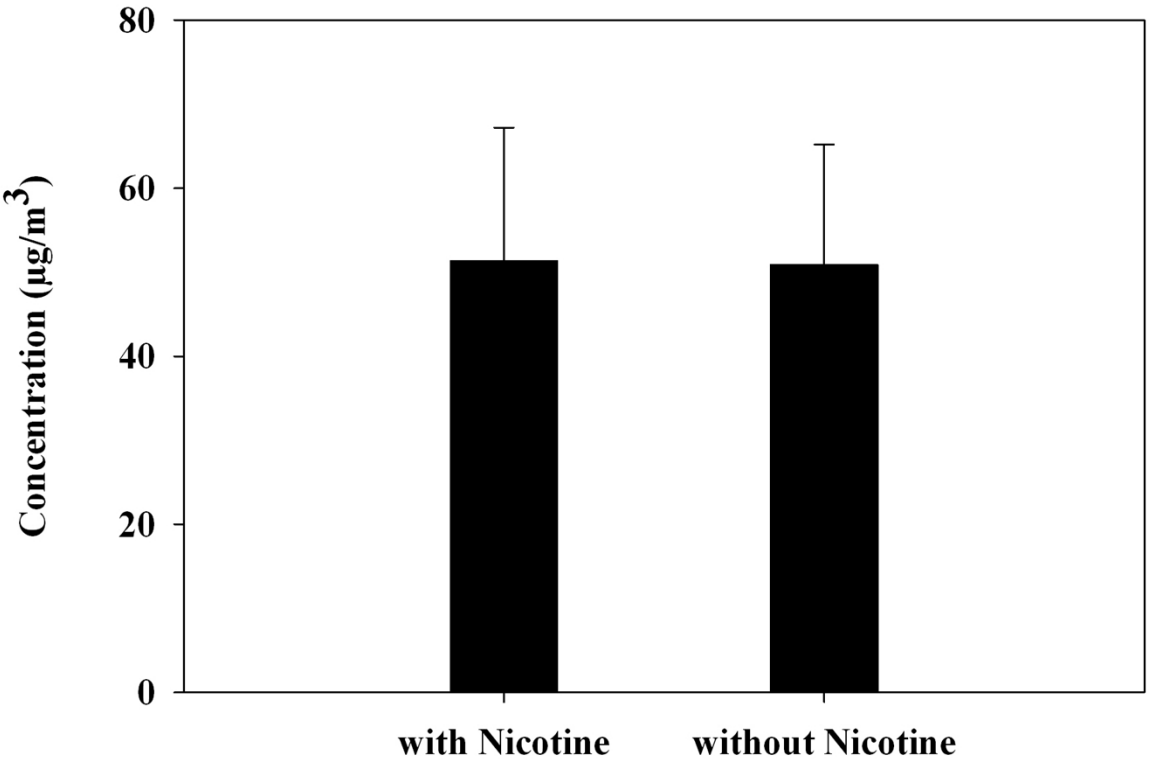

Figure S2. Average total concentration (ng/m^3) of elements as well as organic groups (polycyclic aromatic hydrocarbons (PAHs), hopanes, n-alkanes, organic acids and levoglucosan). Error bars represent analytical uncertainties.

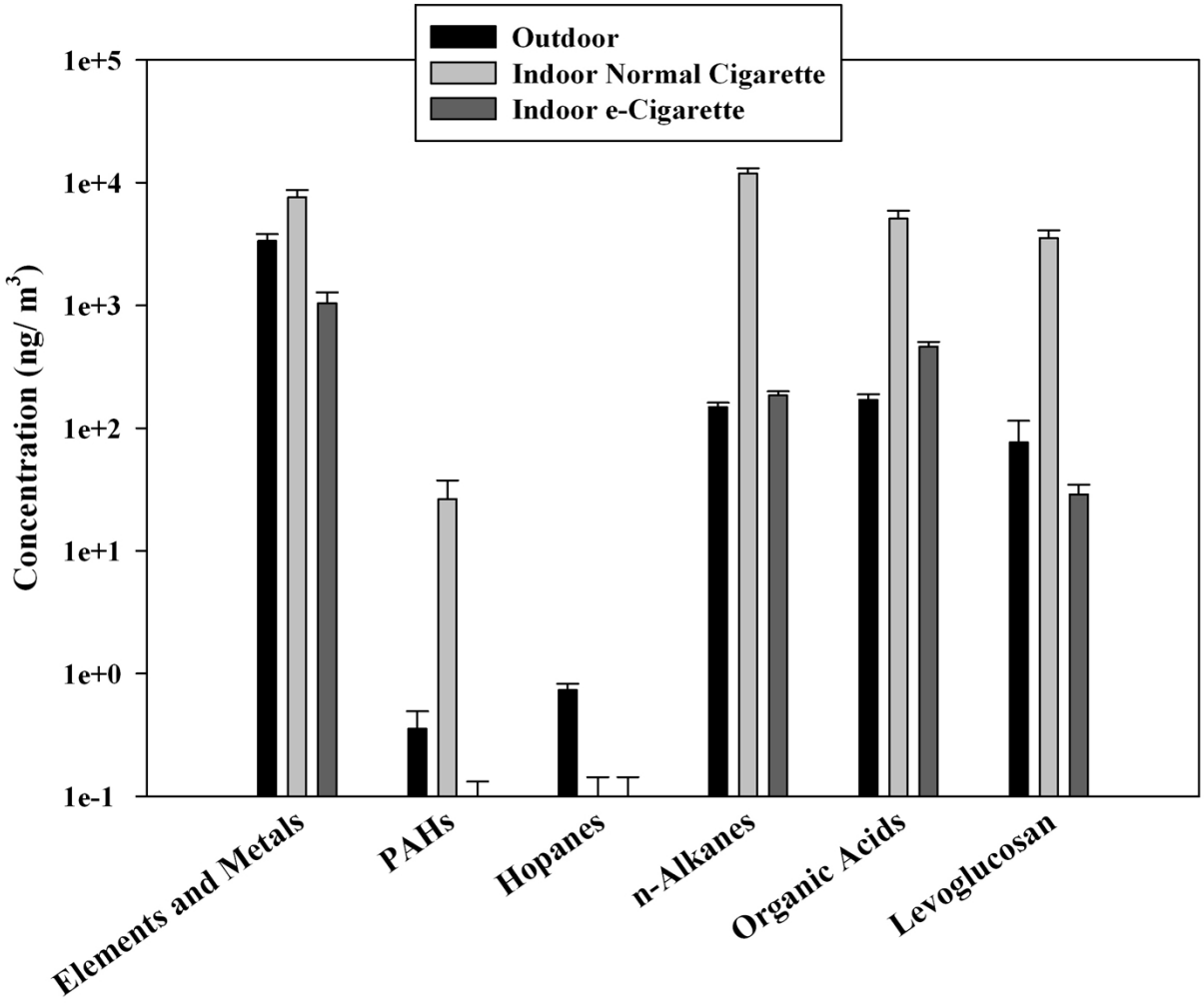

Table S1. Concentration and detection limit of individual chemical species including a) elements and metals, b) PAHs c) hopanes, steranes and levoglucosan d) alkanes and e) organic acids. Concentration values correspond to average ±standard error. "N.D" corresponds to the species that were not detected in the analysis (i.e. species with zero concentration). Values below the limit of detection (LOD) are shown as " < LOD value".

(a) Elements and Metals

Compound	Outdoor (ng/m^3)	Indoor (ng/m^3)		Detection Limit (ng/m^3)
		e-Cigarette	normal-Cigarette	
Li	0.5 (±0.15)	< 0.07	0.4 (±0.2)	0.07
B	6.2 (±1.64)	19.81 (±2.32)	402.66 (±53.03)	1.87
Mg	200.1 (±35.43)	13.3 (±6.43)	96.64 (±94.64)	1.43
Al	333.27 (±62.93)	161.43 (±71.35)	174.22 (±77.62)	1.65
P	3.49 (±0.45)	< 1.11	3.44 (±1.45)	1.11
S	437.2 (±91.97)	236.83 (±34.16)	867.26 (±96.87)	0.10
K	186.4 (±79.14)	267.5 (±42.38)	5111.56 (±987.01)	0.29
Ca	676.2 (±170.08)	10.81 (±0.16)	11.38 (±0.56)	1.67
Sc	0.07 (±0.01)	< 0.04	< 0.04	0.04
Ti	13.81 (±2.61)	8.89 (±1.89)	3.55 (±1.87)	1.80
V	1.34 (±0.29)	0.48 (±0.12)	0.37 (±0.08)	0.17
Cr	5.53 (±1.07)	4.22 (±1.67)	1.61 (±1.49)	0.39
Mn	18.16 (±2.61)	4.73 (±0.75)	8.94 (±1.89)	0.50
Fe	1073 (±152.4)	221.09 (±34)	425.01 (±58.1)	1.93
Co	0.39 (±0.1)	0.15 (±0.08)	0.19 (±0.08)	0.04
Ni	5.57 (±1.65)	6.14 (±2.92)	6.33 (±3.02)	1.03
Cu	39.76 (±4.92)	12.73 (±3.02)	44.86 (±17.63)	0.55
Zn	54.31 (±11.31)	56.01 (±21.45)	190.78 (±111.75)	1.61
Rb	0.74 (±0.14)	0.33 (±0.04)	4.23 (±0.71)	0.03
Sr	3.3 (±0.71)	< 0.24	< 0.24	0.24
Y	< 0.04	< 0.04	< 0.04	0.04
Nb	0.1 (±0.02)	< 0.05	< 0.05	0.05

Mo	**2.79 (±0.46)**	**1.36 (±0.43)**	**2.27 (±1.99)**	**0.47**
Rh	**< 0.54**	**< 0.54**	**< 0.54**	**0.54**
Pd	**< 0.27**	**< 0.27**	**< 0.27**	**0.27**
Ag	**1.84 (±1.66)**	**0.46 (±0.11)**	**0.45 (±0.29)**	**0.06**
Cd	**0.18 (±0.04)**	**0.12 (±0.02)**	**11.14 (±1.09)**	**0.05**
Sn	**9.27 (±2.37)**	**0.95 (±0.55)**	**0.14 (±0.01)**	**0.09**
Sb	**2.59 (±0.44)**	**0.84 (±0.32)**	**1.38 (±0.86)**	**0.13**
Cs	**< 0.12**	**< 0.12**	**< 0.12**	**0.12**
Ba	**6.29 (±5.87)**	**< 1.39**	**4.44 (±3.44)**	**1.39**
La	**0.3 (±0.1)**	**0.24 (±0.11)**	**31.08 (±3.37)**	**0.03**
Ce	**0.57 (±0.12)**	**< 0.10**	**< 0.10**	**0.10**
Pr	**0.06 (±0.01)**	**< 0.03**	**< 0.03**	**0.03**
Nd	**0.23 (±0.05)**	**< 0.07**	**< 0.07**	**0.07**
Sm	**< 0.01**	**< 0.01**	**< 0.01**	**0.01**
Eu	**< 0.06**	**< 0.06**	**< 0.06**	**0.06**
Dy	**< 0.06**	**< 0.06**	**< 0.06**	**0.06**
Ho	**< 0.06**	**< 0.06**	**< 0.06**	**0.06**
Yb	**< 0.02**	**< 0.02**	**< 0.02**	**0.02**
Lu	**< 0.06**	**< 0.06**	**< 0.06**	**0.06**
W	**1.38 (±0.41)**	**0.67 (±0.18)**	**0.3 (±0.13)**	**0.24**
Pt	**< 0.04**	**< 0.04**	**< 0.04**	**0.04**
Tl	**< 0.02**	**< 0.02**	**< 0.02**	**0.02**
Pb	**13.28 (±1.89)**	**9.85 (±2.56)**	**182.22 (±90.39)**	**0.87**
Th	**< 0.03**	**< 0.03**	**< 0.03**	**0.03**
U	**< 0.01**	**< 0.01**	**< 0.01**	**0.01**

(b) PAHs

Compound	Outdoor (ng/m3)	Indoor (ng/m^3)		Detection Limit (ng/m^3)
		e-Cigarette	normal-Cigarette	
Phenanthrene	< 0.41	< 0.41	N.D	0.41
Anthracene	N.D	N.D	N.D	0.03
Fluoranthene	< 0.33	N.D	N.D	0.33
Acephenanthrylene	N.D	N.D	N.D	0.12
Pyrene	0.14 (±0.05)	< 0.06	N.D	0.06
Methylfluoranthene	N.D	N.D	N.D	0.09
Benzo(ghi)fluoranthene	N.D	N.D	N.D	0.03
Cyclopenta(cd)pyrene	N.D	N.D	N.D	0.12
Benz(a)anthracene	N.D	N.D	1.43 (±0.17)	0.25
Chrysene	0.18 (±0.06)	N.D	3.68 (±0.41)	0.10
1-Methylchrysene	N.D	N.D	N.D	0.03
Retene	N.D	N.D	N.D	0.09
Benzo(b)fluoranthene	N.D	N.D	5.12 (±0.75)	0.25
Benzo(k)fluoranthene	N.D	N.D	2.16 (±0.45)	0.06
Benzo(j)fluoranthene	N.D	N.D	N.D	0.03
Benzo (e) pyrene	N.D	N.D	1.75 (±0.48)	0.19
Benzo(a)pyrene	N.D	N.D	4.68 (±0.65)	0.13
Indeno(1,2,3-cd)pyrene	N.D	N.D	4.5 (±0.49)	0.13
Benzo(g,h,i)perylene	0.19 (±0.06)	N.D	3.11 (±0.44)	0.12

(c) Levoglucosan, Hopanes and Steranes

Compound	Outdoor (ng/m^3)	Indoor (ng/m^3)		Detection Limit (ng/m^3)
		e-Cigarette	normal-Cigarette	
Levoglucosan	112.18 (±28)	45.72 (±21.3)	3527.4 (±68.7)	0.79
17A(H)-22,29,30-Trisnorhopane	< 0.17	< 0.17	N.D	0.17
17A(H)-21B(H)-30-Norhopane	0.38 (±0.02)	< 0.13	N.D	0.13
17A(H)-21B(H)-Hopane	0.29 (±0.09)	< 0.17	N.D	0.17
22S-Homohopane	0.28 (±0.08)	N.D	N.D	0.09
22R-Homohopane	0.12 (±0.04)	< 0.09	N.D	0.09
22S-Bishomohopane	N.D	N.D	N.D	0.03
22R-Bishomohopane	N.D	N.D	N.D	0.03
22S-Trishomohopane	N.D	N.D	N.D	0.03
22R-Trishomohopane	N.D	N.D	N.D	0.03
AAA-20S-C27-Cholestane	N.D	N.D	N.D	0.03
ABB-20R-C27-Cholestane	N.D	N.D	N.D	0.03
AAA-20R-27-cholestane	N.D	N.D	N.D	0.03
ABB-20R-C28-Ergostane	N.D	N.D	N.D	0.03
ABB-20S-C28-Ergostane	N.D	N.D	N.D	0.03
ABB-20R-C29-Sitostane	N.D	N.D	N.D	0.03
ABB-20S-C29-Sitostane	N.D	N.D	N.D	0.03

(d) Alkanes

Compound	Outdoor (ng/m^3)	Indoor (ng/m^3)		Detection Limit (ng/m^3)
		e-Cigarette	normal-Cigarette	
n-Tridecane	N.D	N.D	N.D	0.59
n-Tetradecane	< 1.68	< 1.68	< 1.68	1.68
Norpristane	N.D	N.D	N.D	1.68
Pristane	N.D	N.D	N.D	0.31
Phytane	N.D	N.D	N.D	0.59
n-Nonadecane	23.63 (±4.3)	< 0.34	210.45 (±17.66)	0.34
n-Eicosane	22.95 (±3.82)	12.07 (±12.07)	203.19 (±17.93)	1.68
n-Heneicosane	< 0.24	N.D	23.86 (±11.95)	0.24
n-Docosane	19.01 (±3.22)	10.74 (±10.74)	169.53 (±9.9)	1.68
n-Tricosane	2.89 (±0.96)	< 1.68	39.45 (±2.28)	1.68
n-Tetracosane	5.94 (±1.98)	11.52 (±3.45)	89.49 (±2.06)	1.07
n-Pentacosane	2.57 (±0.06)	5.04 (±0.43)	97.73 (±10.79)	0.78
n-Hexacosane	1.64 (±0.07)	3.06 (±0.58)	60.79 (±2.48)	0.24
n-Heptacosane	4.75 (±0.59)	3.92 (±0.26)	848.06 (±53.14)	0.81
n-Octacosane	6.61 (±2.2)	< 1.07	153 (±7.99)	1.07
iso-Nonacosane	N.D	N.D	200.38 (±16.46)	0.88
Nonacosane	9.31 (±1.67)	6.87 (±1.61)	887.98 (±65.05)	1.35
Anteiso-triacontane	N.D	N.D	643.84 (±37.69)	1.07
Triacontane	9.74 (±2.81)	9.23 (±3.85)	391.25 (±23.7)	1.68
iso-Hentriacontane	N.D	N.D	1118.65 (±46.87)	1.51
Hentriacontane	14.32 (±3.15)	13.98 (±5.54)	2767.33 (±74.76)	1.68
Dotriacontane	16.59 (±4.24)	15.88 (±6.84)	599.58 (±16.94)	1.77
Tritriacontane	15.81 (±3.42)	16.03 (±5.24)	1575.82 (±45.3)	1.68
Tetratriacontane	16.13 (±3.34)	16.76 (±5.26)	81.76 (±8.23)	1.07
Pentatriacontane	11.74 (±2.36)	12.37 (±3.24)	67.31 (±2.21)	1.00
Hexatriacontane	10.76 (±1.88)	12.51 (±2.28)	18.73 (±2.08)	0.65
Heptatriacontane	7.32 (±1.01)	8.94 (±1.38)	21.25 (±1.81)	0.51
Octatriacontane	7.24 (±1.01)	9.69 (±1.15)	15.66 (±0.58)	0.08

(e) Organic Acids

Compound	Outdoor (ng/m³)	Indoor (ng/m³)		Detection Limit (ng/m³)
		e-Cigarette	normal-Cigarette	
Octanoic Acid	N.D	< 1.68	N.D	1.68
Decanoic Acid	2.69 (±0.9)	4.38 (±2.88)	22.84 (±4.35)	1.01
Dodecanoic Acid	31.06 (±8.03)	52.07 (±21.72)	206.86 (±1.38)	1.68
Tetradecanoic Acid	45.37 (±7.97)	138.32 (±50.28)	284.03 (±29.41)	1.07
Pentadecanoic Acid	13 (±2.3)	38.87 (±13.15)	133.19 (±12.68)	1.66
Hexadecanoic Acid	74.99 (±3.28)	240.65 (±56.35)	2204.34 (±49.84)	1.68
Heptadecanoic Acid	7.26 (±2.1)	10.97 (±3.35)	137.36 (±2.23)	1.92
Octadecanoic Acid	< 1.68	< 1.68	807.01 (±33.94)	1.68
Nonadecanoic Acid	0.55 (±0.18)	1.34 (±0.47)	27.68 (±2.25)	0.46
Pinonic Acid	7.23 (±0.7)	N.D	N.D	1.65
Palmitoleic Acid	6.87 (±2.29)	29.6 (±9.95)	138.33 (±25.72)	1.68
Oleic Acid	N.D	< 1.68	585.35 (±15.26)	1.68
Linoleic Acid	< 1.07	7.51 (±2.92)	1084.6 (±29.08)	1.07
Eicosanoic Acid	2.07 (±0.6)	3.69 (±1.26)	232.24 (±16.54)	1.20
Heneicosanoic Acid	< 1.06	< 1.06	64.16 (±4.33)	1.06
Docosanoic Acid	3.4 (±0.52)	5.47 (±1.36)	210.9 (±12.57)	0.84
Tricosanoic Acid	2.45 (±0.33)	3.11 (±1.04)	109.19 (±5.9)	0.91
Tetracosanoic Acid	5.98 (±0.92)	10.87 (±2.35)	172.95 (±10.54)	0.66
Pentacosanoic Acid	1.79 (±0.6)	3.77 (±1.28)	47.37 (±2.55)	1.58
Hexacosanoic Acid	3.83 (±0.44)	5.94 (±0.74)	60.07 (±3.45)	0.75
Heptacosanoic Acid	N.D	< 1.22	31.11 (±0.57)	1.22
Octacosanoic Acid	6.51 (±0.35)	7.93 (±0.33)	168.46 (±8.19)	0.83
Nonacosanoic Acid	N.D	N.D	53.12 (±2.01)	1.26
Triacontanoic Acid	6.9 (±0.44)	7.88 (±0.7)	115.83 (±5.2)	1.23
Dehydroabietic Acid	N.D	N.D	N.D	1.07
7-oxodehydroabietic acid	N.D	N.D	N.D	0.61
Phthalic Acid	14.66 (±1.87)	< 1.07	34.36 (±4.19)	1.07
Methylphthalic Acid	2.82 (±0.44)	< 1.37	5.52 (±2.77)	1.37
Succinic Acid	7.32 (±1.58)	< 0.92	225.57 (±51.05)	0.92
Glutaric Acid	3.94 (±1.14)	N.D	36.31 (±1.33)	1.16
Adipic Acid	1.54 (±0.51)	N.D	55.96 (±12.54)	1.20
Pimelic Acid	< 1.68	N.D	N.D	1.68
Suberic Acid	8.35 (±1.16)	10.84 (±4.02)	41.22 (±3.49)	0.53
Azelaic Acid	19.48 (±2.34)	28.1 (±11.62)	93.54 (±8.42)	0.75
Sebacic Acid	< 1.07	N.D	N.D	1.07

I-1 (2-methylglyceric acid)	**N.D**	**N.D**	**N.D**	**1.49**
T-3 (2,3-dihydroxy-4-oxopentanoic Acid)	**N.D**	**N.D**	**N.D**	**1.49**
I-2 (2-methylthreitol)	**N.D**	**N.D**	**N.D**	**1.49**
I-3 (2-Methylthreitol)	**4.21 (±1.4)**	**N.D**	**N.D**	**1.68**
A-5 (3-hydroxyglutaric Acid)	**N.D**	**N.D**	**N.D**	**1.49**
PA (pinic acid)	**N.D**	**N.D**	**N.D**	**1.49**
A-6 (2-hydroxy-4,4-dimethylglutaric Acid)	**N.D**	**N.D**	**N.D**	**1.49**
A-4 (3acetyl hexanedioic acid)	**N.D**	**N.D**	**N.D**	**1.49**
A-3 (2-hydroxy-4-isopropyladipic Acid)	**N.D**	**N.D**	**46.73 (±7.48)**	**1.68**
C-1 (b-carophylinic acid)	**N.D**	**N.D**	**N.D**	**1.49**

Table S2. Average indoor (i.e. inside of the smoking room) to outdoor mass concentration ratio of organic species for normal cigarette samples. Values correspond to average ±standard error.*

Species	I/O Ratio	Species	I/O Ratio
n-Eicosane	8.9 (±0.8)	Tetradecanoic Acid	12.4 (±1.3)
n-Docosane	8.9 (±0.5)	Pentadecanoic Acid	18.6 (±1.8)
n-Tetracosane	15.1 (±0.3)	Hexadecanoic Acid	31.2 (±2.8)
n-Pentacosane	38.1 (±4.2)	Heptadecanoic Acid	19.7 (±1.0)
n-Hexacosane	42.8 (±1.7)	Nonadecanoic Acid	251.3 (±20.4)
n-Heptacosane	302.1 (±18.9)	Palmitoleic Acid	186.9 (±34.7)
Nonacosane	248.3 (±18.2)	Linoleic Acid	1028 (±27.6)
Triacontane	664.8 (±40.3)	Eicosanoic Acid	289.5 (±20.6)
Hentriacontane	768.4 (±20.8)	Docosanoic Acid	119.6 (±7.1)
Dotriacontane	283.7 (±8.0)	Tricosanoic Acid	81.5 (±4.4)
Tritriacontane	371.9 (±10.7)	Tetracosanoic Acid	61.6 (±3.8)
Tetratriacontane	17.2 (±1.7)	Pentacosanoic Acid	125.2 (±6.7)
Pentatriacontane	18.4 (±0.6)	Hexacosanoic Acid	26.0 (±1.5)
Hexatriacontane	4.3 (±0.5)	Octacosanoic Acid	31.1 (±1.5)
Heptatriacontane	5.3 (±0.5)	Triacontanoic Acid	20.0 (±0.9)
Octatriacontane	3.9 (±0.1)	Suberic Acid	7.8 (±0.7)
Decanoic Acid	94.3 (±18.0)	Azelaic Acid	6.1 (±0.6)
Dodecanoic Acid	54.2 (±0.4)	Levoglucosan	225.6 (±4.4)

* Evaluation of correlation coefficients between outdoor and indoor concentrations was not possible due to the small number of data points.

Table S3. Concentration of chemical species in the e-liquid sample (in µg/ml and ng/ml for organics and elements, respectively), including (a) polycyclic aromatic hydrocarbons (PAHs), (b) alkanes, (c) organic acids and (d) elements. Values correspond to average ±analytical uncertainty. Values below the limit of detection (LOD) are shown as " < LOD value".

(a) PAHs	Concentration (µg/ml)
Fluoranthene	< 0.075
Acephenanthrylene	< 0.1
Pyrene	< 0.075
Benzo(ghi)fluoranthene	< 0.125
Cyclopenta(cd)pyrene	< 0.1
Chrysene/triphenylene	< 0.1
Benzo(a)anthracene	< 0.125
Benzo(b)fluoranthene	< 0.235
Benzo(j)fluoranthene	< 0.075
Benzo(k)fluoranthene	< 0.115
Benzo(e)pyrene	< 0.075
Benzo(a)pyrene	< 0.07
Perylene	< 0.19
Indeno(cd)pyrene	< 0.14
Dibenz(ah)anthracene	< 0.05
Benzo(ghi)perylene	< 0.05
Coronene	< 0.1
Dibenzo(ae)pyrene	< 0.1
Retene	< 0.325
1-Methyl chrysene	< 0.05

(b) n-Alkanes	Concentration (µg/ml)	(b) n-Alkanes	Concentration (µg/ml)
Nonane	< 1.0	Triacontane	< 1.0
Decane	< 1.0	Hentriacontane	< 1.0
Undecane	< 1.0	Dotriacontane	< 1.0
Dodecane	< 1.0	Tritriacontane	< 1.0
Tridecane	< 1.0	Tetratriacontane	< 1.0
Tetradecane	< 1.0	Hexatriacontane	< 1.0
Pentadecane	< 1.0	Heptatriacontane	< 1.0
Hexadecane	< 1.0	Octatriacontane	< 1.0
Heptadecane	< 1.0	Nonatriacontane	< 1.0
Octadecane	< 1.0	Tetracontane	< 1.0
Nonadecane	< 1.0	Anteiso-dotriacontane	< 1.0
Eicosane	< 1.0	Anteiso-triacontane	< 1.0
Heneicosane	< 1.0	Iso-hentriacontane	< 1.0
Docosane	< 1.0	Iso-nonacosane	< 1.0
Tricosane	< 1.0	Iso-tritriacontane	< 1.0
Tetracosane	< 1.0	Squalane	< 1.0
Pentacosane	< 1.0	Norpristane	< 1.0
Hexacosane	< 1.0	Phytane	< 1.0
Heptacosane	< 1.0	Pristane	< 1.0
Octacosane	< 1.0		

(c) Organic Acids	Concentration (µg/ml)	(c) Organic Acids	Concentration (µg/ml)
Succinic Acid	< 0.25	Nonacosanoic Acid	< 0.50
Glutaric Acid	< 0.25	Hexadecanoic Acid	511 (±148)
Adipic Acid	< 0.25	Heptadecanoic Acid	< 0.50
Pimelic Acid	< 0.25	Octadecanoic Acid	247 (±118)
Suberic Acid	< 0.25	Nonadecanoic Acid	< 0.50
Azelaic Acid	< 0.25	Eicosanoic Acid	< 0.50
Sebacic Acid	< 0.25	Heneicosanoic Acid	< 0.50
Isophthalic Acid	< 0.25	Docosanoic Acid	< 0.50
Phthalic Acid	< 0.25	Tricosanoic Acid	< 0.50
Terephthalic Acid	< 0.25	Tetracosanoic Acid	< 0.50
Methylphthalic Acid	< 0.25	Pentacosanoic Acid	< 0.50
Benzenetricarboxylic Acid	< 0.25	Triacontanoic Acid	< 0.50
Benzenetetracarboxylic Acid	< 0.25	Palmitoleic Acid	< 0.50
Pinonic Acid	< 0.50	Linoleic Acid	< 0.50
Tetradecanoic Acid	< 0.50	Oleic Acid	< 0.50
Pentadecanoic Acid	< 0.50	Palmitic Acid	< 0.50

(d) Elements	Concentration (ng/ml)
B	**8.91 (±1.94)**
Mg	**109 (±4.89)**
Al	**10.2 (±0.64)**
S	**285 (±22.1)**
K	**1743 (±182)**
Ca	**285 (±6.93)**
Ti	**55.8 (±3.8)**
V	**1.61 (±0.19)**
Cr	**2.37 (±0.17)**
Mn	**1.84 (±0.44)**
Fe	**39.1 (±6.88)**
Co	**0.09 (±0.02)**
Cu	**0.54 (±0.06)**
Zn	**2.88 (±0.41)**
Rb	**4.2 (±0.41)**
Mo	**0.77 (±0.05)**
Ag	**0.04 (±0.02)**
Cd	**0.08 (±0.03)**
Sn	**0.18 (±0.02)**
Sb	**1.02 (±0.07)**
La	**0.02 (±0.005)**
W	**0.97 (±0.11)**
Pb	**0.16 (±0.02)**