

Table 1. Compounds identified in tobacco and electronic cigarettes.

N	RT (min)	Compound	No smoking		Tobacco		e-cigarette Type 1		e-cigarette Type 2	
			Indoor air	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath
1	3.768	Sulfur dioxide + Difluorodimethylsilane	✓	✓	✓	✓	✓	✓	-	✓
2	4.098	Butene isomer	-	-	-	✓	-	-	-	-
3	4.164	Buta-1,3-diene	-	-	-	✓	-	-	-	-
4	4.259	Butene isomer	-	-	-	✓	-	-	-	-
5	4.387	Butene isomer	-	-	-	✓	-	-	-	-
6	4.675	Ethanol	✓	✓	-	✓	-	✓	-	-
7	4.762	Isopropylethylene	-	-	-	✓	-	-	-	-
8	4.993	iso-Pentane	-	-	-	✓	-	-	-	-
9	5.100	Penta-1,4-diene	-	-	-	✓	-	-	-	-
10	5.273*	<i>Pent-1-ene</i>	✓	✓	✓	✓	-	✓	-	-
11	5.327	Acetone	✓	✓	-	✓	-	✓	-	✓
12	5.393*	<i>Pent-2-ene</i>	-	-	✓	✓	-	-	-	-
13	5.409	Isopropanol	✓	-	-	-	-	-	-	✓
14	5.413*	<i>n-Pentane</i>	-	-	✓	✓	-	✓	-	✓
15	5.677*	<i>Isoprene</i>	✓	✓	✓	✓	-	✓	✓	✓
16	5.797*	<i>Pent-2-ene</i>	✓	✓	✓	✓	-	✓	-	-
17	5.912	iso-Pentene	-	-	✓	✓	-	-	-	-
18	6.118	Pentadiene	-	-	✓	✓	-	-	-	-
19	6.176	Methyl acetate	-	-	-	✓	-	-	-	-
20	6.456	Pentadiene	-	✓	✓	✓	-	-	-	-
21	6.514	Cyclopenta-1,3-diene	-	-	-	✓	-	-	-	-
22	6.518	Unknown	-	-	-	-	-	✓	-	✓
23	7.025	Cyclopentene	-	-	-	✓	-	-	-	-
24	7.041	Propan-1-ol	-	-	-	✓	-	✓	-	✓
25	7.351	2-Methylpent-2-ene	-	-	✓	✓	-	-	-	-
26	7.618	Methacrolein	-	-	✓	-	-	-	-	-
27	7.623	2-Methylpenta-1,4-diene	-	-	-	✓	-	-	-	-
28	7.932	Propanenitrile	-	-	-	✓	-	-	-	-
29	7.994	3-Methylpentane	-	-	-	✓	-	-	-	-
30	8.229	Acetic acid	✓	✓	-	-	-	✓	-	✓
31	8.303	Unknown (m/z=155)	-	-	-	-	-	✓	-	✓
32	8.286	Methyl vinyl ketone	-	-	-	✓	-	-	-	-
33	8.356	Hex-1-ene	-	-	-	✓	-	-	-	-
34	8.468	Butane-2,3-dione	-	-	-	✓	-	-	-	-
35	8.744	Methyl ethyl ketone	-	-	-	✓	-	-	-	-
36	8.736*	<i>n-Hexane</i>	✓	✓	✓	✓	✓	✓	-	✓
37	9.053	Methylfuran	-	-	✓	✓	-	✓	-	✓
38	9.168	Methylpentene	-	-	✓	✓	-	-	-	-
39	9.407	Methylpentene	-	-	✓	✓	-	-	-	-
40	9.483	Unknown	✓	✓	-	-	-	✓	-	✓
41	9.506	trans-2-Methylpenta-1,3-diene	-	-	✓	✓	-	-	-	-
42	9.630	Methylfuran	-	-	✓	✓	-	-	-	-
43	10.005	Methylpent-2-ene isomer	-	-	✓	✓	-	-	-	-
44	10.018	Dimethyl carbonate	-	-	-	-	✓	-	-	-
45	10.434	Hexadiene	-	-	✓	✓	-	-	-	-
46	10.562	Isobutyronitrile	-	-	✓	✓	-	-	-	-
47	11.118	Hexadiene	-	-	-	✓	-	-	-	-
48	11.407	Methyl-1,3-cyclopentadiene	-	-	✓	✓	-	✓	-	✓
49	11.691	Methyl-1,3-cyclopentadiene	-	-	✓	✓	-	✓	-	✓
50	12.111	Methylcyclopentene	-	-	✓	✓	-	-	-	-
51	12.243	Methylcyclopentene	-	-	✓	✓	-	-	-	-
52	12.371	Crotonaldehyde	-	-	✓	✓	-	-	-	-
53	12.717	Isovaleraldehyde	-	-	✓	✓	-	-	-	-
54	12.869*	<i>Benzene</i>	✓	✓	✓	✓	✓	✓	✓	✓
55	12.969	Unknown	-	-	-	-	✓	-	-	-
56	12.270	2-Methylbutanal	-	-	✓	-	✓	✓	-	-
57	13.385	Methyl-1,3-cyclopentadiene	-	-	✓	✓	-	-	-	-

Table 1 (continued)

N	RT (min)	Compound	No smoking		Tobacco		e-cigarette Type 1		e-cigarette Type 2	
			Indoor air	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath
58	13.496	Branched heptane	-	-	-	-	-	-	-	✓
59	13.612	Methyl propenyl ketone	-	-	✓	-	-	-	-	-
60	14.317*	Isooctane	✓	✓	-	-	-	✓	✓	✓
61	14.374	Methyl propyl ketone	-	-	✓	✓	-	-	-	-
62	14.510	Hept-1-ene	-	-	✓	✓	-	-	-	-
63	15.017*	<i>n</i> -Heptane	✓	✓	✓	✓	-	✓	✓	✓
64	15.046	Allyl methyl sulfide	-	✓	-	-	-	✓	-	-
65	15.170	Pentane-2,3-dione	-	-	-	-	-	-	-	-
66	15.215	cis-3-Methylhex-2-ene	-	-	-	✓	-	-	-	-
67	15.252	Unknown	-	-	✓	-	-	-	-	-
68	15.524	2,5-dimethylfuran	-	✓	✓	✓	-	✓	-	✓
69	16.687	Vinylfuran	-	-	✓	-	-	-	-	-
70	16.823	Hepta-1,5-diene	-	-	✓	-	-	-	-	-
71	17.231	3-methylbutanenitrile	-	-	✓	✓	-	-	-	-
72	17.367	(E)-1-(methylthio)prop-1-ene	-	-	-	-	-	✓	-	-
73	(17.5-23.5)	Propylene glycol	-	-	-	-	✓	-	✓	-
74	17.544	Methyl propenyl ketone	-	-	✓	✓	-	-	-	-
75	17.566	1-Methyl-1H-pyrrole	-	-	✓	✓	-	-	-	-
76	17.705	1-Methyl-1,4-cyclohexadiene	-	-	✓	✓	-	-	-	-
77	18.039	Pyridine	-	-	-	✓	-	-	-	-
78	18.282	Pyrrole	-	-	-	✓	-	-	-	-
79	19.263*	Toluene	✓	✓	✓	✓	-	✓	✓	✓
80	20.277	Unknown (m/z=229, m/z=73)	✓	✓	-	-	-	✓	-	✓
81	20.285	Oct-2-ene	-	-	✓	-	-	-	-	-
82	20.603	Cyclopentanone	-	-	-	-	-	-	-	-
83	20.735*	<i>n</i> -Octane	✓	✓	✓	✓	-	✓	-	✓
84	20.838	C ₁₂ H ₂₂ O	-	-	✓	-	-	-	-	-
85	21.180	Hexamethylcyclotrisiloxane	✓	✓	✓	✓	✓	✓	-	✓
86	21.555	Butyl Acetate	-	-	-	-	✓	-	-	-
87	21.588	2,5-Dimethyl-2,4-hexadiene	-	-	✓	-	-	-	-	-
88	21.876	Methylpyridine	-	-	✓	✓	-	-	-	-
89	22.116	C ₃ H ₁₀ N ₂	-	-	-	-	✓	-	-	-
90	22.251	Methylpyrazine	-	-	✓	✓	-	-	-	-
91	22.396	Cresol isomer	-	-	✓	-	-	-	-	-
92	22.643	Furfural	-	-	✓	✓	-	-	-	-
93	22.680	Cyclopentenone	-	-	✓	✓	-	-	-	-
94	23.138	2-Methylcyclopentanone	-	-	✓	✓	-	-	-	-
95	24.044*	Ethylbenzene	✓	✓	✓	✓	✓	✓	-	✓
96	24.127	Methylpyridine	-	-	✓	✓	-	-	-	-
97	24.374	Unknown (m/z=289)	✓	✓	-	-	-	✓	-	✓
98	24.436*	<i>m</i> -Xylene	✓	✓	✓	✓	✓	✓	✓	✓
99	24.510*	<i>p</i> -Xylene	✓	✓	✓	✓	✓	✓	✓	✓
100	24.704	Unknown	-	-	✓	-	-	-	✓	-
101	25.215	1,2-Propanediol, 2-acetate	-	-	-	-	-	-	✓	-
102	25.236	1,6-Dimethylhepta-1,3,5-triene	-	-	-	-	-	-	-	-
103	25.475	Styrene	✓	✓	✓	✓	-	-	-	-
104	25.516*	<i>o</i> -Xylene	✓	✓	✓	✓	✓	✓	✓	✓
105	25.697	cis-2,6-Dimethyl-2,6-octadiene	-	-	✓	-	-	-	-	-
106	25.990	2-Methyl-2-cyclopenten-1-one	-	-	✓	✓	-	-	-	-
107	27.313	3,4-Dimethyl-2-cyclopenten-1-one	-	-	✓	✓	-	-	-	-
108	28.117	Octamethylcyclotetrasiloxane	✓	✓	-	✓	✓	✓	✓	✓
109	28.228	Limonene isomer	-	-	✓	✓	-	-	-	-
110	28.303	1-Ethyl-2-methylbenzene	-	-	✓	✓	-	-	-	-
111	28.509	1-Ethyl-3-methylbenzene	-	-	✓	-	-	-	-	-
112	28.500	Glycerin	-	-	-	-	-	✓	-	-
113	28.587	Benzaldehyde	✓	✓	-	✓	-	✓	-	✓
114	28.682	Phenol	✓	✓	-	✓	-	✓	-	✓
115	28.727	4-Ethenylpyridine	-	-	✓	✓	-	-	-	-
116	(29.5-34.5)	Glycerin	-	-	-	-	✓	-	✓	-

N	RT (min)	Compound	No smoking		Tobacco		e-cigarette Type 1		e-cigarette Type 2	
			Indoor air	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath
117	29.139	(Z)-(cis-Geraniol)	-	-	✓	✓	-	-	-	-
118	29.444	Benzonitrile	-	-	-	✓	-	-	-	-
119	29.473	Unknown	-	-	✓	-	-	-	-	-
120	29.692	Trimethylbenzene	-	-	✓	✓	-	-	-	-
121	29.716	Unknown	-	-	✓	✓	-	-	-	-
122	29.741	Octanal	✓	✓	-	-	-	-	-	-
123	29.981	δ-Camphene	-	-	✓	✓	-	-	-	-
124	30.607	2-Ethylhexan-1-ol,	-	✓	-	-	-	-	-	-
125	30.788	m-Cymene	-	✓	✓	✓	-	-	-	-
126	30.974	δ-Limonene	✓	✓	✓	✓	-	✓	-	✓
127	31.246	Eucalyptol	-	✓	-	-	-	-	-	-
128	31.258	Ocimene	-	-	✓	✓	-	-	-	-
129	31.839	Indene	-	-	✓	-	-	-	-	-
130	32.470	Acetophenone	✓	✓	-	-	-	-	-	-
131	33.233	Nonanal	✓	✓	-	-	-	-	-	-
132	33.331	Decamethylcyclopentasiloxane	✓	✓	-	-	-	✓	-	✓
133	33.509	Unknown	-	✓	-	-	-	-	-	-
134	34.428	Unknown	✓	✓	-	-	-	-	-	-
135	34.551	Benzoic acid	✓	✓	-	✓	✓	✓	-	✓
136	35.203	2,3-dimethylphenol	-	-	✓	-	-	-	-	-
137	35.607	Decanal	-	✓	-	✓	-	✓	-	✓
138	35.809*	<i>Naphthalene</i>	✓	-	✓	✓	-	-	-	-
139	36.332	2,3-Dihydrobenzofuran	-	-	✓	-	-	-	-	-
140	36.435	Nonanoic acid	✓	✓	-	✓	-	✓	-	✓
141	36.773	Dodecamethylcyclohexasiloxane	✓	✓	-	✓	✓	✓	-	✓
142	37.791	Hydroquinone	-	-	✓	-	-	-	-	-
143	37.931	Unknown	-	-	✓	-	-	-	-	-
144	38.228	Decanoic acid	-	-	✓	-	-	✓	-	-
145	38.813*	<i>Nicotine</i>	-	-	✓	✓	✓	✓	✓	✓
146	39.702	Vanillin	-	-	-	-	-	-	✓	-
147	39.762	7-methyl-1H-indole	-	-	✓	-	-	-	-	-
148	39.815	Tetradecamethylcycloheptasiloxane	-	-	-	✓	-	✓	-	✓
149	40.729	Myosmine	-	-	✓	-	✓	-	-	-
150	40.887	Ethyl Vanillin	-	-	-	-	-	-	✓	-
151	41.641	Nicotyrine	-	-	✓	✓	✓	✓	✓	-
152	42.585	Dimethylaminocinnamitrile	-	-	-	-	✓	-	-	-
153	43.723	Isonicotine	-	-	✓	-	✓	-	-	-
154	43.888	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	-	-	-	✓	-	✓	-	-
155	43.933	Hexadecamethylheptasiloxane	-	-	-	-	✓	-	-	-
156	44.424	Dimethylaminocinnamitrile	-	-	-	-	✓	-	-	-

*compounds quantified

Table 2. Figures of merit.

Compound	Range ^a (ng)	R ²	RSD ^b (%)	LOD ^c (ng)	Bio-VOC		
					Mean ^d (ng)	Repeatability (RSD %)	Recovery (%)
Pent-1-ene	0.5-10	0.9962	7.1	0.17	10.4	17.7	94
	10-250	0.9971					
n-Pentane	0.25-10	0.9997	5.5	0.05	12.6	22.7	109
	10-250	0.9971					
Pent-2-ene	0.5-10	0.9984	4.7	0.12	11.8	18.1	103
	10-250	0.9966					
Isoprene	0.25-10	0.9982	4.5	0.11	10.7	19.3	92
	10-250	0.9969					
Pent-2-ene	0.25-10	0.9994	4.1	0.06	11.1	18.6	97
	10-250	0.9966					
n-Hexane	1-30	0.9977	4.5	0.43	11.5	17.6	89
	30-250	0.9965					
Benzene	0.25-10	0.9962	3.5	0.16	13.6	12.4	99
	10-250	0.9955					
Isooctane	0.6-26	0.9996	3.1	0.13	37.5	13.8	114
	26-260	0.9977					
n-Heptane	0.5-10	0.9983	3.2	0.11	22.4	14.8	96
	10-470	0.9920					
Toluene	1-25	0.9989	6.1	0.65	12.8	18.3	110
	25-250	0.9812					
n-Octane	0.5-10	0.9977	4.8	0.13	23.6	11.2	96
	10-200	0.9975					
Ethylbenzene	0.25-5	0.9987	4.0	0.05	11.5	6.5	92
	5-100	0.9990					
m-Xylene	0.25-5	0.9965	3.2	0.08	11.4	7.5	92
	5-100	0.9988					
p-Xylene	0.25-5	0.9979	4.5	0.06	11.3	5.9	97
	5-100	0.9983					
o-Xylene	0.25-5	0.9987	4.1	0.05	11.4	6.1	94
	5-100	0.9987					
Naphthalene	0.25-5	0.9978	6.3	0.06	10.6	8.5	92
	5-50	0.9989					

^aAmount introduced into the cartridges. ^bResidual standard deviation of the calibration lines. ^cLimits of detection.

^dMean values of replicate analyses for calculation of repeatability and recovery

Table 3. Concentrations ($\mu\text{g}/\text{m}^3$) of selected VOC in air, smoke and exhaled breath^a.

Compound	No smoking		Tobacco cigarette smoking		Type 1 e-cigarette smoking		Type 2 e-cigarette smoking	
	Indoor air	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath	Smoke	Exhaled breath
Pent-1-ene	0.5	0.6	700	68	nd	0.3	nd	nd
n-Pentane	nd	nd	1200	63	nd	7	nd	nd
Pent-2-ene	nd	0.5	625	52	nd	0.3	nd	nd
Isoprene	0.4	87	2700	670	nd	47	nd	45
Pent-2-ene	nd	0.3	460	32	nd	0.2	nd	nd
n-Hexane	1	nd	975	14	nd	nd	nd	0.6
Benzene	0.6	4	1100	49	0.6	0.8	nd	0.5
Isooctane	0.4	0.2	nd	nd	nd	0.2	nd	1.5
n-Heptane	0.2	0.4	890	26	nd	0.3	1	2.1
Toluene	5	11	1400	60	nd	3	4	6.4
n-Octane	nd	0.2	560	3	nd	nd	nd	nd
Ethylbenzene	0.2	0.6	660	6	1	0.2	nd	0.3
m-Xylene	0.2	0.5	980	7	nd	0.2	nd	0.2
p-Xylene	0.1	0.2	420	2	0.6	0.1	nd	0.1
o-Xylene	0.1	0.2	590	2	0.4	0.1	nd	0.1
Naphthalene	0.05	0.1	240	3	nd	nd	nd	nd
Nicotine	nd	nd	1300	7	720	4	710	1

^aall compounds were quantified with authentic standards except nicotine that was quantified with naphthalene.