

## Supplementary Table S1 (Foods)

### Insights on single-dose espresso coffee capsules' volatile profile: from ground powder volatiles to prediction of espresso brew aroma properties

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**Table S1.** Chromatographic details and aroma descriptors of 390 volatile compounds putatively identified in 8 capsule-coffee powders and espresso brews using HS-SPME/GC × GC-ToFMS.

Peak num	<sup>1</sup> t <sub>R</sub> (s) <sup>a</sup>	<sup>2</sup> t <sub>R</sub> (s) <sup>a</sup>	Compound	CAS number	Formula	RI <sub>Calc</sub> <sup>b</sup>	RI <sub>Lit</sub> <sup>c</sup>	RI Ref.	Previously reported <sup>d</sup>	Aroma descriptor <sup>e</sup>	Aroma descriptor Ref.
<b>Acids</b>											
<i>Aliphatics</i>											
1	144	5.370	Acetic acid	64-19-7	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	672	648	[1]	[91]	Pungent, sour, acidic, vinegar	[109, 114-116]
2	180	1.660	Propanoic acid	79-09-4	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	721	699	[2]	[91]	Pungent, rancid, sour milk, cheese, butter-like	[114, 116]
3	270	2.980	Butanoic acid	107-92-6	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	828	815	[1]	[91]	Sour, rancid, butter-like, sweaty, rubbish	[98, 114, 116, 117]
4	342	2.030	Isovaleric acid	503-74-2	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	880	880	[3]	[91]	Acidic, cheesy, herbaceous, sweaty, rancid	[98, 114-116, 118]
<b>Alcohols</b>											
<i>Aliphatics</i>											
5	108	0.850	2-Methyl-1-propanol	78-83-1	C <sub>4</sub> H <sub>10</sub> O	610	612	[4]	[91]	Wine-like	[116]
6	114	1.240	3-Buten-1-ol	627-27-0	C <sub>4</sub> H <sub>8</sub> O	620	-	-	-	-	-
7	174	1.460	3-Methyl-3-buten-1-ol	763-32-6	C <sub>5</sub> H <sub>10</sub> O	711	708	[4]	[91]	-	-
8	180	1.180	2-Methyl-1-butanol	137-32-6	C <sub>5</sub> H <sub>12</sub> O	720	728	[1]	[92]	Cooked, roasted with fruity or alcoholic undertones	[116]
9	210	1.340	1-Pentanol	71-41-0	C <sub>5</sub> H <sub>12</sub> O	766	767	[3]	[91]	Green, chemical, fusel oil-like sweet	[114, 116, 119]
10	222	1.800	3-Methyl-2-buten-1-ol	556-82-1	C <sub>5</sub> H <sub>10</sub> O	785	782	[2]	[91]	Fresh, herbaceous-fruity-green, lavender-like, phenolic, metallic	[114, 116]
11	246	1.060	2-Hexanol	626-93-7	C <sub>6</sub> H <sub>14</sub> O	809	813	[5]	[91]	-	-
12	384	1.110	2-Heptanol	543-49-7	C <sub>7</sub> H <sub>16</sub> O	908	906	[2]	[91]	Fresh, lemon-like, grassy-herbaceous, sweet-floral undertone	[114, 116]
13	516	1.360	1-Octen-3-ol	3391-86-4	C <sub>8</sub> H <sub>16</sub> O	984	980	[4]	[91]	Mushroom, herbaceous, savoury, brothy, meaty	[98, 119, 120]
14	600	1.280	2-Ethyl-1-hexanol	104-76-7	C <sub>8</sub> H <sub>18</sub> O	1032	1033	[2]	[93]	Sweet, slightly floral rose-like	[116]
15	678	1.360	1-Octanol	111-87-5	C <sub>8</sub> H <sub>18</sub> O	1077	1079	[4]	[94]	Fresh, orange-rose, sweet	[116]
<i>Aromatics</i>											
16	756	4.550	2-Phenylethanol	60-12-8	C <sub>8</sub> H <sub>10</sub> O	1124	1121	[2]	[91]	Rose-honey-like, floral	[114, 116, 119]
<b>Aldehydes</b>											
<i>Aliphatics</i>											
17	66	0.350	Acetaldehyde	75-07-0	C <sub>2</sub> H <sub>4</sub> O	546	548	[4]	[91]	Pungent, ethereal, fruity, coffee, wine, acrid/egg,	[114, 116, 119, 121, 122]
18	90	0.430	2-Methylpropanal	78-84-2	C <sub>4</sub> H <sub>8</sub> O	582	582	[6]	[91]	Pungent, sour, fruity, malty, buttery-oily	[114, 116, 123]
19	120	0.710	2-Butenal	4170-30-3	C <sub>4</sub> H <sub>6</sub> O	628	633	[4]	[95, 96]	-	-
20	126	0.460	3-Methylbutanal	590-86-3	C <sub>5</sub> H <sub>10</sub> O	637	633	[4]	[91]	Pungent, acrid, fruity, apple-like, almond, malty, sweaty	[114, 116, 118, 121, 123]
21	180	0.770	2-Methyl-2-butenal	1115-11-3	C <sub>5</sub> H <sub>8</sub> O	719	715	[7]	[91]	-	-
22	192	0.850	2-Pentenal	764-39-6	C <sub>5</sub> H <sub>8</sub> O	738	726	[8]	-	Pungent, green, apple, orange, tomato	[116]
23	240	0.660	Hexanal	66-25-1	C <sub>6</sub> H <sub>12</sub> O	805	801	[4]	[91]	Fatty, green, grassy, fruity, rancid butter-like, nutty	[114, 116, 117, 119, 123]
24	258	0.800	4-Methyl-3-pentenal	5362-50-5	C <sub>6</sub> H <sub>10</sub> O	818	-	-	-	-	-
25	336	0.750	2-Methyl-2-hexenal	28467-88-1	C <sub>7</sub> H <sub>12</sub> O	874	884	[9]	-	-	-
26	336	1.350	2,4-Hexadienal	80466-34-8	C <sub>6</sub> H <sub>8</sub> O	875	879	[10]	[91]	Fresh, green, floral, citrus	[116]
27	342	0.690	4-Methylhexanal	41065-97-8	C <sub>7</sub> H <sub>14</sub> O	879	889	[9]	-	-	-
28	378	0.710	Heptanal	111-71-7	C <sub>7</sub> H <sub>14</sub> O	904	906	[3]	[91]	Oily-fatty, rancid, pungent, fermented-fruit-like	[114, 116]
29	474	0.960	2-Heptenal	2463-63-0	C <sub>7</sub> H <sub>12</sub> O	959	959	[4]	[94]	Pungent, green, fatty	[116]
30	552	0.740	Octanal	124-13-0	C <sub>8</sub> H <sub>16</sub> O	1004	1001	[4]	[91]	Fatty, citrus, orange-like, honey	[116, 126]
31	594	1.310	2,4-Heptadienal	5910-85-0	C <sub>7</sub> H <sub>10</sub> O	1028	1043	[11]	[97]	Fatty, green ((E,E)-isomer)	[116]
32	648	1.000	2-Octenal	2363-89-5	C <sub>8</sub> H <sub>14</sub> O	1059	1059	[2]	[98]	Green-leafy, orange, honey-like, cognac-like	[98, 116]
33	726	0.770	Nonanal	124-19-6	C <sub>9</sub> H <sub>18</sub> O	1104	1106	[4]	[94, 99]	Fatty, orange and rose note, soap-like, metallic	[116, 125]
34	822	0.950	2-Nonenal	2463-53-8	C <sub>9</sub> H <sub>16</sub> O	1161	1162	[4]	[91]	Fatty, orris-like, waxy, dried orange peels-like, cardboard-like	[116, 117]
35	900	0.780	Decanal	112-31-2	C <sub>10</sub> H <sub>20</sub> O	1208	1207	[4]	[97, 99, 100]	Sweet, waxy, floral, citrus, fatty	[116]
36	1068	0.730	Undecanal	112-44-7	C <sub>11</sub> H <sub>22</sub> O	1309	1307	[4]	[100]	Sweet, fatty, orange and rose undertone	[116]
37	1224	0.780	Dodecanal	112-54-9	C <sub>12</sub> H <sub>24</sub> O	1413	1407	[4]	[97, 100]	Fatty, violet-like	[116]
<i>Aromatics</i>											
38	474	2.150	Benzaldehyde	100-52-7	C <sub>7</sub> H <sub>6</sub> O	960	965	[4]	[91]	Sweet, bitter almond-like, bitter	[114, 116, 119]
39	618	2.380	Benzeneacetaldehyde	122-78-1	C <sub>8</sub> H <sub>8</sub> O	1043	1046	[4]	[91]	Pungent-green, hyacinth-like, floral, sweet-fruity, honey-like	[114, 116, 118, 124, 125]
40	618	2.750	2-Hydroxybenzaldehyde	90-02-8	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	1043	1044	[2]	[91]	Pungent, herbaceous, spicy-floral, bitter, almond-like	[114, 116]
41	660	1.960	2-Methylbenzaldehyde	529-20-4	C <sub>8</sub> H <sub>8</sub> O	1067	1074	[4]	[91]	Sweet, beany, fresh pea	[98, 114]
42	1008	2.260	2-Phenyl-2-butenal	4411-89-6	C <sub>10</sub> H <sub>10</sub> O	1273	1278	[2]	[91]	Musty, floral, cocoa	[128]
<b>Esters</b>											
<i>Aliphatics</i>											
43	84	0.420	Methyl acetate	79-20-9	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	573	566	[3]	[91]	Sweet, ethereal, fruity	[114, 116]
44	102	0.500	Methyl propenoate	96-33-3	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	601	607	[12]	-	-	-
45	108	0.470	Methyl propanoate	554-12-1	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	610	615	[13]	[91]	Ethereal-um-like, sweet, fruity	[114, 116]
46	150	3.410	Methyl glycolate	96-35-5	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	678	-	-	[95]	-	-
47	156	0.570	Methyl 2-methylpropenoate	80-62-6	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	683	685	[4]	-	Acrid, fruity	[116]
48	162	0.540	Methyl butanoate	623-42-7	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	692	720	[13]	[91]	Sweet-ethereal, fruity, apple peel, peach-like	[114, 116]

49	198	0.770	Methyl 2-butenote	18707-60-3	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	747	755	[14]	[96]	-	
50	210	0.530	Methyl 2-methylbutanoate	868-57-5	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	764	770	[15]		Sweet, fruity, apple-like	[116]
51	216	0.570	Methyl 3-methylbutanoate	556-24-1	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	774	775	[12]	[91]	Ethereal, fruity, apple-like, herbaceous	[114, 116]
52	228	0.650	3-Methylbutyl formate	110-45-2	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	792	791	[2]	[98]	Plum, fruity, black currant-like	[98, 116]
53	258	0.620	Butyl acetate	123-86-4	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	818	818	[4]	[91]	Pear-like, ethereal, fruity, ripe/over-ripe fruits-like	[114, 116]
54	270	0.610	Methyl pentanoate	624-24-8	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	827	829	[5]		Ethereal, green-fruity, apple-like, pineapple-like	[114, 116]
55	294	0.810	Methyl 3-methyl-2-butenote	924-50-5	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	844	842	[16]	[101]	roasted	[129]
56	312	0.570	Ethyl 3-methylbutanoate	108-64-5	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	857	857	[3]	[91]	Fruity, apple-like	[116, 117, 119]
57	348	0.630	Isoamyl acetate	123-92-2	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	883	882	[3]	[91]	Fruity, banana, sweet, apple-like	[114, 116]
58	354	0.620	Methyl 3-methylpentanoate	2177-78-8	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	887	-	-		-	
59	360	0.780	3-Methyl-3-butenyl acetate	5205-07-2	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	892	881	[17]		Fruity	[116]
60	366	0.630	Methyl 4-methylpentanoate	2412-80-8	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	896	900	[18]		Sweet, pineapple-like	[116]
61	402	0.660	Pentyl acetate	628-63-7	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	918	916	[3]		-	
62	420	0.660	Methyl hexanoate	106-70-7	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	928	927	[3]	[91]	Pineapple-like, apricot-like, sweet, ethereal	[114, 116]
63	420	0.750	Ethyl tiglate	5837-78-5	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	928	929	[19]		Fruity, caramel	[114, 116]
64	420	0.820	3-Methyl-2-butenyl acetate	1191-16-8	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	928	929	[20]	[91]	Fresh, fruity, banana-like, bergamot-like	[114]
65	426	0.730	Hexyl formate	629-33-4	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	931	927	[21]		Fruity, apple-like, unripe-plum	[116]
66	456	1.530	Ethylidene acetate	542-10-9	C <sub>8</sub> H <sub>10</sub> O <sub>4</sub>	949	-	-		-	
67	504	1.190	Methyl 4-methyl-2-oxopentanoate	3682-43-7	C <sub>7</sub> H <sub>12</sub> O <sub>3</sub>	977	-	-		-	
68	516	0.640	Butyl 2-methyl-2-propenoate	97-88-1	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	983	989	[22]		-	
69	570	0.680	Hexyl acetate	142-92-7	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	1014	1006	[3]	[102]	Fruity, apple, cherry, pear, floral	[116]
70	684	0.710	Isobutyl 3-methyl-2-butenote	30434-54-9	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	1080	-	-		-	
71	768	0.720	Methyl octanoate	111-11-5	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	1129	1130	[3]		Winy, fruity, orange-like	[116]
72	864	0.720	3-Methylbutyl 3-methyl-2-butenote	56922-73-7	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	1186	1184	[23]		-	
73	1092	0.680	Methyl decanoate	110-42-9	C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>	1325	1332	[3]		-	
74	1392	0.680	Methyl dodecanoate	111-82-0	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	1531	1527	[5]		Fatty, floral, wine-like	[116]
<b>Aromatics</b>											
75	654	1.990	Phenyl acetate	122-79-2	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	1063	1068	[18]	[103, 104]	Floral, rosy, dark chocolate-like	[128]
76	678	2.310	Benzyl formate	104-57-4	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	1077	1077	[5]	[91]	Fruity, green, herbaceous, earthy, floral	[114, 116]
77	708	1.710	Methyl benzoate	93-58-3	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	1094	1096	[2]	[91]	Fruity, cananga-like	[116]
78	852	1.920	Methyl phenylacetate	101-41-7	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	1180	1179	[5]	[91]	Honey, musky, jasmine, floral	[114, 116]
79	852	2.110	2-Phenylethyl formate	104-62-1	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	1180	1176	[5]	[91]	Green, herbaceous, rosy, hyacinth, chrysanthemum, watercress-	[114, 116]
80	882	1.880	Methyl 2-hydroxybenzoate	119-36-8	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	1198	1207	[3]	[91]	Sweet, rooty-fruity, minty, spicy, wintergreen-like	[114, 116]
81	990	1.540	2-Phenylethyl acetate	103-45-7	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	1262	1260	[4]	[105]	Floral, rose, honey-like	[116]
82	1002	1.550	Ethyl 2-hydroxybenzoate	118-61-6	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	1269	1280	[24]	[96]	Wintergreen	[116]
<b>Furan compounds</b>											
83	78	0.380	Furan	110-00-9	C <sub>4</sub> H <sub>4</sub> O	564	567	[25]	[91]	Spicy-smokey, cinnamon-like	[114]
84	102	0.460	2-Methylfuran	534-22-5	C <sub>5</sub> H <sub>6</sub> O	601	601	[26]	[91]	Ethereal, sickly	[109]
85	108	0.420	Tetrahydrofuran	109-99-9	C <sub>4</sub> H <sub>8</sub> O	610	634	[27]	[91]	Sweet-gassy, bread-like	[114]
86	150	0.500	2,5-Dimethylfuran	625-86-5	C <sub>6</sub> H <sub>8</sub> O	703	704	[28]	[91]	coffee	[109]
87	174	0.580	2,4-Dimethylfuran	3710-43-8	C <sub>6</sub> H <sub>8</sub> O	710	735	[29]	[96]	-	
88	228	0.570	2-Propylfuran	4229-91-8	C <sub>7</sub> H <sub>10</sub> O	792	788	[12]	[91]	-	
89	240	0.570	2-Ethyl-5-methylfuran	1703-52-2	C <sub>7</sub> H <sub>10</sub> O	805	799	[28]	[91]	-	
90	246	0.470	2-Ethyl-5-methyltetrahydrofuran	931-39-5	C <sub>7</sub> H <sub>14</sub> O	809	-	-		-	
91	246	2.470	2-Furancarboxitrile	617-90-3	C <sub>5</sub> H <sub>5</sub> NO	810	822	[30]		-	
92	252	1.290	Dihydro-2-methyl-3-furanone	3188-00-9	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	814	813	[2]	[91]	Bread-like, buttery, nutty	[109, 116]
93	258	0.590	2,3,5-Trimethylfuran	10504-04-8	C <sub>7</sub> H <sub>10</sub> O	818	817	[31]	[91]	-	
94	264	2.840	3-Furaldehyde	498-60-2	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	824	831	[32]	[91]	-	
95	276	0.760	2-Vinyl-5-methylfuran	10504-13-9	C <sub>7</sub> H <sub>8</sub> O	831	841	[31]	[91]	Coffee	[109]
96	276	1.100	2-(Methoxymethyl)furan	13679-46-4	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	831	-	-	[91]	Burnt, herbal, potato-like	[98, 126]
97	282	0.630	2,3,4-Trimethylfuran	10599-57-2	C <sub>7</sub> H <sub>10</sub> O	835	-	-	[91]	-	
98	282	3.300	Furfural	98-01-1	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	837	839	[1]	[91]	Sweet, bread-like, caramellic, cinnamon-almond-like, bitter	[109, 114]
99	312	0.900	2-(2-Propenyl)furan	75135-41-0	C <sub>7</sub> H <sub>8</sub> O	857	856	[28]	[91]	-	
100	336	2.190	5-Methyl-2(3H)-furanone	591-12-8	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	876	874	[33]	[98, 106]	Sweet, herbaceous, tobacco-like, coffee, earthy, raw potato skin	[98, 109, 116]
101	342	2.010	2-Furanmethanol	98-00-0	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	880	867	[3]	[91]	Slightly caramellic, warm, oily, burnt, bitter	[98, 114, 116, 119]
102	360	0.470	2,5-Diethyltetrahydrofuran	41239-48-9	C <sub>8</sub> H <sub>16</sub> O	892	896	[16]		Sweet, herbaceous, caramellic	[116]
103	366	0.610	2-Butylfuran	4466-24-4	C <sub>8</sub> H <sub>12</sub> O	896	898	[29]	[91]	-	
104	390	2.700	Furfuryl formate	13493-97-5	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	912	902	[34]	[91]	Floral	[109]
105	402	2.530	2-Acetylfuran	1192-62-7	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	919	917	[2]	[91]	Balsamic-sweet, tobacco-like, floral, balsamic-cinnamic, spicy,	[109, 114, 116, 126]
106	414	4.220	γ-Butyrolactone	96-48-0	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	927	924	[4]	[91]	Sweet, slightly buttery	[109, 114, 116]
107	432	0.660	2,3,4,5-Tetramethylfuran	10599-58-3	C <sub>8</sub> H <sub>12</sub> O	935	-	-	[91]	-	
108	450	1.100	3-(1,1-Dimethylethyl)-2,3-dihydrofuran	34314-82-4	C <sub>8</sub> H <sub>14</sub> O	945	-	-		-	
109	468	2.200	1-(2-Furyl)-2-propanone	6975-60-6	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	956	963	[26]	[91]	Sweet, fruity-caramellic, spicy, radish	[114, 116]

110	474	0.840	2-Methyl-5-propenylfuran	5555-95-3	C <sub>8</sub> H <sub>10</sub> O	959	972	[31]	[91]	Candy, fruity, sweet	[98]
111	480	3.090	Dihydro-5-methyl-2(3H)-furanone	108-29-2	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	964	965	[30]	[91]	Sweet, hay-like, tobacco-like, herbaceous	[114, 116]
112	486	2.700	5-Methylfurfural	620-02-0	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	967	965	[3]	[91]	Sweet, spicy, caramel	[109, 114, 116, 119]
113	504	1.610	2-Acetyl-5-methylfuran	1193-79-9	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	977	977	[35]	[91]	Nutty	[116]
114	510	2.510	Methyl 2-furoate	611-13-2	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	981	983	[36]	[91]	Berry-like, fruity, winey, mushrooms-like, fungus-like, tobacco-like	[114, 116]
115	534	0.660	2-Pentylfuran	3777-69-3	C <sub>9</sub> H <sub>14</sub> O	993	992	[36]	[91]	Fruity, green bean, metallic, vegetable	[116]
116	534	1.670	Benzofuran	271-89-6	C <sub>8</sub> H <sub>6</sub> O	994	996	[3]	[91]	-	
117	540	1.940	Furfuryl acetate	623-17-6	C <sub>7</sub> H <sub>8</sub> O <sub>3</sub>	998	998	[37]	[91]	Ethereal-floral, herbal-spicy, fruity, banana, nutty	[109, 114, 116]
118	552	2.930	2,5-Dihydro-3,5-dimethyl-2-furanone	5584-69-0	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	1005	993	[38]	[99, 107]	-	
119	564	2.070	1-(2-Furanyl)-1-propanone	3194-15-8	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	1012	1014	[27]	[91]	-	
120	612	2.030	2,2'-Bifuran	5905-00-0	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	1039	1044	[28]	[91]	-	
121	624	1.670	3,4-Dimethyl-2,5-furandione	766-39-2	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	1046	1046	[27]	[91]	-	
122	630	1.720	1-(5-Methyl-2-furyl)-2-propanone	13678-74-5	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	1049	1047	[39]	[91]	-	
123	642	1.810	1-(2-Furanyl)-2-butanone	4208-63-3	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	1056	1063	[26]	[91]	-	
124	648	2.100	5-Ethyl-2-furaldehyde	23074-10-4	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	1060	1058	[27]	[91]	-	
125	678	2.050	1-(2-Furanyl)-3-butanone	699-17-2	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	1077	1077	[33]	[91]	-	
126	690	1.720	2,2'-Methylenebisfuran	1197-40-6	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	1084	1084	[33]	[91]	-	
127	696	1.480	3-Acetyl-2,5-dimethylfuran	10599-70-9	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	1087	1089	[27]		-	
128	702	1.580	Furfuryl propanoate	623-19-8	C <sub>8</sub> H <sub>10</sub> O <sub>3</sub>	1091	1096	[28]	[91]	Spicy, floral, fruity	[116, 130]
129	720	1.810	1-(2-Furanyl)-1-butanone	4208-57-5	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	1101	-	-	[91]	-	
130	732	1.410	2-Methylbenzofuran	4265-25-2	C <sub>9</sub> H <sub>8</sub> O	1108	1108	[27]	[91]	-	
131	774	1.730	2-Methyl-5-propionylfuran	10599-69-6	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	1133	1136	[27]	[91]	-	
132	798	1.450	1-(5-Methyl-2-furanyl)-2-butanone	13678-70-1	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	1147	-	-	[91]	-	
133	834	2.220	2-Heptylfuran	3777-71-7	C <sub>11</sub> H <sub>18</sub> O	1169	1154	[3]	[91]	Roasted, nutty	[116]
134	846	1.410	Furfuryl butanoate	623-21-2	C <sub>9</sub> H <sub>12</sub> O <sub>3</sub>	1173	1171	[40]	[91]	-	
135	858	1.430	2-(2-Furanylmethyl)-5-methylfuran	13678-51-8	C <sub>10</sub> H <sub>10</sub> O <sub>2</sub>	1183	1179	[33]	[91]	-	
136	864	2.410	<i>n</i> -Furfuryl pyrrole	1438-94-4	C <sub>8</sub> H <sub>9</sub> NO	1187	1189	[28]	[91]	Vegetable, green, earthy, horseradish, mushroom-like	[116, 130]
137	876	2.640	2-Methyl-3(2-furyl)acrolein	874-66-8	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	1194	1196	[25]		-	
138	876	2.970	4-(2-Furanyl)-3-buten-2-one	623-15-4	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	1195	1191	[25]	[91]	Spicy-woody, sweet, cinnamon-like, balsamic, vanilla, woody	[109, 116]
139	906	1.340	4,7-Dimethylbenzofuran	28715-26-6	C <sub>10</sub> H <sub>10</sub> O	1212	1218	[25]		-	
140	990	2.780	2-Furyl pyrazine	32736-95-1	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O	1262	-	-	[91]	-	
141	1020	1.220	2,2'-Methylenebis(5-methylfuran)	13679-43-1	C <sub>11</sub> H <sub>12</sub> O <sub>2</sub>	1279	1277	[33]	[91]	-	
142	1020	1.870	1-(5-Methylfurfuryl)pyrrole	13678-52-9	C <sub>10</sub> H <sub>11</sub> NO	1280	-	-	[91]	Mushroom-like, green, pharmaceutical, roasty	[126, 130]
143	1056	2.410	Difurfuryl ether	4437-22-3	C <sub>10</sub> H <sub>10</sub> O <sub>3</sub>	1302	1305	[28]	[91]	-	
144	1152	1.700	1-Furfuryl-2-formylpyrrole	13788-32-4	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>	1365	-	-	[91]	green, minty	[109]
145	1326	2.540	2-Acetyl-1-furfurylpyrrole	13678-73-4	C <sub>11</sub> H <sub>11</sub> NO <sub>2</sub>	1485	-	-	[91]	-	

## Hydrocarbons

<i>Aliphatics</i>											
146	378	0.380	Nonane	111-84-2	C <sub>9</sub> H <sub>20</sub>	904	900	[4]	[91]	-	
147	420	0.500	1,3-Nonadiene	-	C <sub>9</sub> H <sub>16</sub>	928	930	[41]		-	
148	546	0.400	Decane	124-18-5	C <sub>10</sub> H <sub>22</sub>	1000	1000	[4]	[91]	-	
149	720	0.410	Undecane	1120-21-4	C <sub>11</sub> H <sub>24</sub>	1100	1101	[2]	[91]	-	
150	882	0.750	1-Dodecene	112-41-4	C <sub>12</sub> H <sub>24</sub>	1197	1192	[42]		-	
151	894	0.430	Dodecane	112-40-3	C <sub>12</sub> H <sub>26</sub>	1204	1201	[4]	[91]	-	
152	1056	0.460	Tridecane	629-50-5	C <sub>13</sub> H <sub>28</sub>	1300	1301	[4]	[91]	-	
153	1212	0.470	Tetradecane	629-59-4	C <sub>14</sub> H <sub>30</sub>	1405	1401	[4]	[91]	-	
154	1356	0.450	Pentadecane	629-62-9	C <sub>15</sub> H <sub>32</sub>	1505	1501	[4]	[91]	-	
155	1494	0.470	Hexadecane	544-76-3	C <sub>16</sub> H <sub>34</sub>	1605	1601	[4]	[91]	-	

## Aromatics

156	204	0.600	Methylbenzene	108-88-3	C <sub>7</sub> H <sub>8</sub>	755	759	[4]	[91]	Sweet-gassy	[114]
157	318	0.680	Ethylbenzene	100-41-4	C <sub>8</sub> H <sub>10</sub>	861	860	[4]	[91]	Sweet-gassy	[114]
158	330	0.690	1,3-Dimethylbenzene	108-38-3	C <sub>8</sub> H <sub>10</sub>	870	871	[4]	[91]	-	
159	360	0.950	Phenylethylene	100-42-5	C <sub>8</sub> H <sub>8</sub>	892	895	[2]	[91]	Sweet-gassy, balsamic, floral	[114, 116]
160	414	0.640	1-Methylethylbenzene	98-82-8	C <sub>9</sub> H <sub>12</sub>	925	927	[4]		-	
161	474	0.690	1-Ethyl-4-methylbenzene	622-96-8	C <sub>9</sub> H <sub>12</sub>	959	964	[4]	[91]	-	
162	582	0.820	1,2,3-Trimethylbenzene	526-73-8	C <sub>9</sub> H <sub>12</sub>	1021	1021	[2]		-	
163	630	0.700	1-Methyl-3-propylbenzene	1074-43-7	C <sub>10</sub> H <sub>14</sub>	1049	1056	[4]		-	
164	642	0.690	Butylbenzene	104-51-8	C <sub>10</sub> H <sub>14</sub>	1056	1054	[21]		-	
165	678	0.740	4-Ethyl-1,2-dimethylbenzene	934-80-5	C <sub>10</sub> H <sub>14</sub>	1076	1082	[43]		-	
166	690	0.780	1-Ethyl-2,3-dimethylbenzene	933-98-2	C <sub>10</sub> H <sub>14</sub>	1083	1085	[2]		-	
167	750	0.820	1,2,4,5-Tetramethylbenzene	95-93-2	C <sub>10</sub> H <sub>14</sub>	1118	1123	[4]	[91]	-	
168	804	0.870	1,2,3,4-Tetramethylbenzene	488-23-3	C <sub>10</sub> H <sub>14</sub>	1151	1150	[44]	[108]	-	
169	816	0.690	Pentylbenzene	538-68-1	C <sub>11</sub> H <sub>16</sub>	1158	1154	[21]		-	

170	1542	0.600	1-Butylheptylbenzene	4537-15-9	C <sub>17</sub> H <sub>28</sub>	1641	1633	[11]	-	
<b>Ketones</b>										
<i>Aliphatics</i>										
171	78	0.410	2-Propanone	67-64-1	C <sub>3</sub> H <sub>6</sub> O	564	559	[4]	[91]	Ethereal, lemon [114, 119]
172	96	0.500	2-Butanone	78-93-3	C <sub>4</sub> H <sub>8</sub> O	592	590	[4]	[91]	Ethereal, sweet apricot-like [114, 116]
173	96	0.600	2,3-Butanedione (Diacetyl)	431-03-8	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	592	591	[4]	[91]	Buttery [114-116, 121, 123]
174	138	0.560	2-Pentanone	107-87-9	C <sub>5</sub> H <sub>10</sub> O	655	664	[4]	[91]	Ethereal-fruity, wine [114, 116]
175	144	0.710	2,3-Pentanedione	600-14-6	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	665	665	[4]	[91]	Buttery, oily, sweet, caramel-like, milky [98, 109, 114-116, 121, 126]
176	168	1.910	1-Hydroxy-2-propanone	116-09-6	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	703	698	[45]	[91]	Sweet-caramellic, mushroom, earthy, nutty [98, 109, 114]
177	180	0.560	4-Methyl-2-pentanone	108-10-1	C <sub>6</sub> H <sub>12</sub> O	719	721	[2]	[91]	Ethereal-fruity, spicy [114, 116]
178	180	0.860	3-Penten-2-one	625-33-2	C <sub>5</sub> H <sub>8</sub> O	719	717	[4]	[91]	Fruity [116]
179	192	1.660	3-Hydroxy-2-butanone (Acetoin)	513-86-0	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	739	733	[46]	[91]	Creamy-fatty-buttery, woody, yogurt [109, 114, 116, 119]
180	204	0.640	2-Methyl-1-penten-3-one	25044-01-3	C <sub>6</sub> H <sub>10</sub> O	756	748	[47]		-
181	216	0.910	2,4-Pentanedione	123-54-6	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	774	783	[36]	[91]	Ethereal-minty, metallic [114]
182	222	0.620	3-Hexanone	589-38-8	C <sub>6</sub> H <sub>12</sub> O	783	785	[18]	[91]	Ethereal, grape, wine-like [98]
183	222	0.770	2,4-Dimethyl-3-pentanone	565-80-0	C <sub>7</sub> H <sub>14</sub> O	783	793	[48]	[91]	-
184	228	0.670	2-Hexanone	591-78-6	C <sub>6</sub> H <sub>12</sub> O	792	791	[2]	[91]	-
185	240	0.790	3,4-Hexanedione	4437-51-8	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	805	804	[28]	[91]	Buttery, toasty, burnt, nutty, caramel-eggy [114, 116]
186	240	2.220	1-Hydroxy-2-butanone	5077-67-8	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	806	-	-	[91]	Toasted [109]
187	258	1.750	3-Hydroxy-2-pentanone	3142-66-3	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	819	807	[2]	[91]	Earthy, aged [98]
188	264	1.870	2-Hydroxy-3-pentanone	5704-20-1	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	823	821	[49]	[91]	-
189	294	0.930	3-Hexen-2-one	763-93-9	C <sub>6</sub> H <sub>10</sub> O	844	845	[50]		-
190	294	1.010	3-Hexene-2,5-dione	4436-75-3	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	844	-	-		-
191	300	0.650	4-Methyl-2-hexanone	105-42-0	C <sub>7</sub> H <sub>14</sub> O	848	848	[2]		-
192	336	0.660	4-Heptanone	123-19-3	C <sub>7</sub> H <sub>14</sub> O	874	871	[4]	[91]	Ethereal-fruity, pineapple-like, strawberry-like [114]
193	354	2.540	1-(Acetyloxy)-2-propanone	592-20-1	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	889	882	[28]	[91]	Fruity-buttery, sour [114]
194	360	0.660	3-Heptanone	106-35-4	C <sub>7</sub> H <sub>14</sub> O	892	889	[4]	[91]	Green, fatty, fruity, sweet, ethereal [114, 116]
195	366	0.720	2-Heptanone	110-43-0	C <sub>7</sub> H <sub>14</sub> O	896	895	[2]	[91]	Fruity, spicy, cinnamon, banana, spicy [116]
196	444	0.940	3-Hepten-2-one	1119-44-4	C <sub>7</sub> H <sub>12</sub> O	942	942	[51]	[98]	Green-grassy [116]
197	444	2.180	2,5-Hexanedione	110-13-4	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	943	949	[25]	[91]	Sweet-ethereal [114]
198	468	0.660	6-Methyl-3-heptanone	624-42-0	C <sub>8</sub> H <sub>16</sub> O	956	941	[52]		-
199	468	0.720	6-Methyl-2-heptanone	928-68-7	C <sub>8</sub> H <sub>16</sub> O	956	955	[53]		-
200	486	0.740	5-Methyl-2-heptanone	18217-12-4	C <sub>8</sub> H <sub>16</sub> O	966	971	[54]		-
201	510	0.820	1-Octen-3-one	4312-99-6	C <sub>8</sub> H <sub>14</sub> O	980	980	[4]	[91]	Mushroom [116, 117, 122, 127]
202	522	0.850	2,3-Octanedione	585-25-1	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	987	985	[4]	[91]	Warmed-over [116]
203	522	0.900	6-Methyl-5-hepten-2-one	110-93-0	C <sub>8</sub> H <sub>14</sub> O	987	985	[4]	[91]	Strong, fatty, green, citrus-like [116]
204	534	0.740	2-Octanone	111-13-7	C <sub>8</sub> H <sub>16</sub> O	994	990	[4]	[91]	Floral, bitter-green, musty-herbaceous, unripe-apple fruity [114, 116]
205	618	0.990	3-Octen-2-one	1669-44-9	C <sub>8</sub> H <sub>14</sub> O	1042	1040	[4]	[91]	Fruity, lemon [116]
206	708	0.780	2-Nonanone	821-55-6	C <sub>9</sub> H <sub>18</sub> O	1093	1095	[4]	[91]	Fruity-floral, fatty, herbaceous, rue [116, 130]
207	792	0.930	3-Nonen-2-one	14309-57-0	C <sub>9</sub> H <sub>16</sub> O	1143	1144	[55]		Fruity [116]
<i>Cyclics</i>										
208	294	1.780	2-Cyclopenten-1-one	930-30-3	C <sub>5</sub> H <sub>6</sub> O	845	835	[32]	[91]	-
209	366	1.070	Cyclohexanone	108-94-1	C <sub>6</sub> H <sub>10</sub> O	896	895	[4]		Peppermint, acetone-like [116]
210	366	4.250	4-Cyclopentene-1,3-dione	930-60-9	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	899	911	[31]	[109, 110]	-
211	390	1.390	2-Methyl-2-cyclopenten-1-one	1120-73-6	C <sub>6</sub> H <sub>8</sub> O	911	920	[31]	[91]	-
212	432	1.640	2-Cyclohexen-1-one	930-68-7	C <sub>6</sub> H <sub>8</sub> O	935	927	[56]	[91]	Gassy-mint [114]
213	486	1.380	5-Ethylcyclopent-2-en-1-one	34094-63-8	C <sub>7</sub> H <sub>10</sub> O	966	966	[57]		-
214	510	1.300	6-Methylenebicyclo[3.2.0]hept-3-en-2-one	-	C <sub>8</sub> H <sub>8</sub> O	980	-	-		-
215	534	1.270	3-Methyl-2-cyclohexen-1-one	1193-18-6	C <sub>7</sub> H <sub>10</sub> O	994	-	-	[91]	Caramel-like, phenolic, mild cherry [116, 130]
216	600	0.750	2,2,6-Trimethylcyclohexanone	2408-37-9	C <sub>9</sub> H <sub>16</sub> O	1032	1036	[5]		-
217	600	3.800	2-Cyclohexene-1,4-dione	4505-38-8	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	1033	1036	[25]		-
218	612	1.040	3,5-Dimethyl-2-cyclohexen-1-one	1123-09-7	C <sub>8</sub> H <sub>12</sub> O	1039	-	-		-
219	612	5.470	2-Hydroxy-3-methyl-2-cyclopenten-1-one	80-71-7	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	1041	1042	[58]	[91]	Sweet, caramellic-spicy, walnut, maple, licorice, celery, tobacco [114, 115, 124]
220	654	1.200	2,3,4-Trimethyl-2-cyclopenten-1-one	28790-86-5	C <sub>8</sub> H <sub>12</sub> O	1063	1071	[28]	[28]	-
221	654	3.990	3,5-Dimethyl-1,2-cyclopentanedione	13494-07-0	C <sub>7</sub> H <sub>10</sub> O <sub>2</sub>	1064	-	-	[91]	-
222	708	2.120	3-Ethyl-2-hydroxy-2-cyclopenten-1-one	21835-01-8	C <sub>7</sub> H <sub>10</sub> O <sub>2</sub>	1094	1091	[59]	[91]	Caramel-like, sweet, sugary [116, 130]
<i>Aromatics</i>										
223	660	2.190	Acetophenone	98-86-2	C <sub>8</sub> H <sub>8</sub> O	1067	1065	[2]	[91]	Sweet [116]
224	768	2.140	1-Phenyl-2-propanone	103-79-7	C <sub>9</sub> H <sub>10</sub> O	1130	1131	[2]		-
225	822	2.320	<i>o</i> -Hydroxyacetophenone	118-93-4	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	1162	1167	[60]	[91]	Sweet, heavy-floral, herbaceous, new-mown hay-like, mimosa -like [114]
226	834	2.340	1-Phenyl-1,2-propanedione	579-07-7	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	1169	1175	[61]	[91]	Warm-floral, herbaceous, plastic [114, 116]
227	864	1.950	<i>p</i> -Methylacetophenone	122-00-9	C <sub>9</sub> H <sub>10</sub> O	1187	1190	[2]		Fruity, floral [116]
228	936	1.710	1-Phenyl-2-butanone	1007-32-5	C <sub>10</sub> H <sub>12</sub> O	1230	1231	[2]		-

229	990	1.860	1-(4-Hydroxyphenyl)-1-propanone	70-70-2	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	1262	-	-	-	-
230	1068	2.470	4-Hydroxy-3-methylacetophenone	876-02-8	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	1310	1311	[33]	[111]	-
<b>Volatile phenols</b>										
231	708	4.560	2-methoxyphenol (Guaiacol)	90-05-1	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	1096	1090	[27]	[91]	Smoke-like, phenolic, burnt, spicy, woody, meaty, sweet
232	738	4.980	2,6-Dimethylphenol	576-26-1	C <sub>8</sub> H <sub>10</sub> O	1114	1108	[48]	[91]	Ground-coffee, phenolic
233	876	1.540	2-Allylphenol	1745-81-9	C <sub>9</sub> H <sub>10</sub> O	1194	1170	[62]		-
234	1020	3.090	4-Ethyl-2-methoxyphenol (4-Ethylguaiacol)	2785-89-9	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	1280	1290	[3]	[91]	Smoky, clove-like, spicy, burnt, vanilla-like, sweet, ethereal, green
235	1080	4.670	2-Methoxy-4-vinylphenol (4-Vinylguaiacol)	7786-61-0	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	1319	1322	[3]	[91]	Spicy, clove-like, phenolic, apple, rum, roasted peanut
<b>Oxazoles</b>										
236	120	0.750	4-Methyloxazole	693-93-6	C <sub>4</sub> H <sub>5</sub> NO	628	-	-		-
237	198	0.890	4,5-Dimethyloxazole	20662-83-3	C <sub>6</sub> H <sub>7</sub> NO	747	750	[63]	[91]	-
238	312	0.850	Trimethyloxazole	20662-84-4	C <sub>6</sub> H <sub>9</sub> NO	857	852	[63]	[91]	-
239	426	0.780	4-Ethyl-2,5-dimethyloxazole	30408-61-8	C <sub>7</sub> H <sub>11</sub> NO	931	919	[39]	[91]	-
240	570	0.730	2-Ethyl-4-methyl-5-propyloxazole	102586-53-8	C <sub>9</sub> H <sub>15</sub> NO	1014	-	-		-
241	588	0.760	4,5-Dimethyl-2-propyloxazole	53833-32-2	C <sub>8</sub> H <sub>13</sub> NO	1025	-	-	[91]	-
242	660	0.710	4,5-Dimethyl-2-isobutyloxazole	26131-91-9	C <sub>9</sub> H <sub>15</sub> NO	1066	-	-		-
243	696	3.000	Benzoxazole	273-53-0	C <sub>7</sub> H <sub>5</sub> NO	1088	-	-	[91]	-
244	744	1.830	2-Methylbenzoxazole	95-21-6	C <sub>8</sub> H <sub>7</sub> NO	1115	-	-	[91]	Sweet, gassy-pungent, floral-sweet, tobacco
<b>Pyrazines</b>										
245	180	1.230	Pyrazine	290-37-9	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	720	729	[28]	[91]	Pungent, sweet, floral, coffee
246	270	1.250	Methylpyrazine	109-08-0	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>	827	833	[28]	[91]	Nutty, cocoa, green, roasted, chocolate, meaty, toasted
247	402	1.120	2,5-Dimethylpyrazine	123-32-0	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	918	912	[28]	[91]	Chocolate, roasted nuts, earthy, grassy, roasted, nutty
248	402	1.170	2-Ethylpyrazine	13925-00-3	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	918	922	[2]	[91]	Peanut butter, musty, nutty, woody, buttery, roasted, green, sweet
249	414	1.190	2,3-Dimethylpyrazine	5910-89-4	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub>	925	922	[2]	[91]	Nutty, cocoa-like odor, green note, toasted, roasted
250	432	1.660	Vinylpyrazine	4177-16-6	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub>	935	935	[12]	[91]	-
251	492	1.020	2-Isopropylpyrazine	9820-90-0	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	970	-	-		-
252	540	1.040	2-Ethyl-6-methylpyrazine	13925-03-6	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	997	1000	[28]	[91]	Toasted, flowery, fruity, hazelnut-like
253	552	1.080	2-Ethyl-3-methylpyrazine	15707-23-0	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	1004	1001	[28]	[91]	Raw-potato, roasted, earthy, nutty, peanut-like, coffee-like
254	564	1.100	2-Propylpyrazine	18138-03-9	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	1011	1010	[63]	[91]	Green, vegetable, herbal
255	576	1.410	2-Vinyl-6-methylpyrazine	13925-09-2	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub>	1018	1020	[12]	[91]	Coffee
256	588	2.470	Acetylpyrazine	22047-25-2	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O	1026	1023	[28]	[91]	Toasted
257	636	0.920	2-Methyl-3-isopropylpyrazine	15986-81-9	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>	1052	1053	[2]		-
258	654	1.000	Isobutylpyrazine	29460-92-2	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>	1063	-	-		-
259	672	1.710	Isopropenylpyrazine	38713-41-6	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub>	1073	1075	[63]	[91]	-
260	684	0.940	2,6-Diethylpyrazine	13067-27-1	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>	1080	1080	[12]	[91]	Toasted, potato-like, roasted
261	714	0.880	2-Isopropyl-3-methoxypyrazine	25773-40-4	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O	1097	1094	[64]	[91]	Vegetable-like, earthy, bell pepper, raw potato, galbanum, roasty
262	732	1.670	6,7-Dihydro-5H-cyclopentapyrazine	23747-47-9	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub>	1108	1104	[65]	[91]	Green, phenolic, nutty, roast
263	756	1.970	2-Acetyl-3-methylpyrazine	23787-80-6	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O	1123	1128	[28]	[91]	Cereal, roasted bean, roasted, nutty, grain-roasted potato
264	780	0.930	2-Isobutyl-3-methylpyrazine	13925-06-9	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub>	1136	1134	[28]	[91]	Herbaceous green earthy notes, green bell peppers
265	786	1.390	5H-5-Methyl-6,7-dihydrocyclopentapyrazine	23747-48-0	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub>	1140	1149	[28]	[91]	Earthy, baked potato, peanut, roasted, nutty
266	792	1.350	2-Methyl-6-(1-propenyl)pyrazine (isomer)	104638-11-1	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub>	1144	-	-	[91]	-
267	816	0.830	2,3-Diethyl-5-methylpyrazine	18138-04-0	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub>	1158	1153	[12]	[91]	Nutty, meaty, roasted hazelnut, earthy, roasty
268	822	1.450	2-Methyl-6-(1-propenyl)pyrazine (isomer)	104638-11-1	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub>	1162	-	-	[91]	-
269	834	0.860	2-Acetyl-3-ethylpyrazine	32974-92-8	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O	1168	1172	[28]	[28]	-
270	852	1.010	2-Isoamylpyrazine	40790-22-5	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub>	1179	-	-		-
271	858	0.880	2-Isobutyl-3-methoxypyrazine	24683-00-9	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O	1183	1181	[64]	[91]	Green bell-pepper note, galbanum oil, red pepper, green, earthy
272	870	0.940	2-Butyl-3-methylpyrazine	15987-00-5	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub>	1190	-	-	[91]	-
273	894	0.830	2,5-Dimethyl-3-isobutylpyrazine	32736-94-0	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub>	1204	1207	[2]	[91]	-
274	894	1.950	1-Methylpyrrolo(1,2-a)pyrazine	64608-59-9	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub>	1205	1214	[28]	[91]	-
275	924	1.160	6,7-Dihydro-2,5-dimethyl-5H-cyclopentapyrazine	38917-61-2	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub>	1222	1220	[31]	[91]	-
276	942	0.770	2,5-Diethyl-3,6-dimethylpyrazine	18903-30-5	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub>	1233	1225	[66]	[91]	-
277	972	0.910	2-Methyl-6-isopentylpyrazine	91010-41-2	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub>	1251	1257	[28]		-
278	1062	0.780	2,6-Dimethyl-3(2-methyl-1-butyl)pyrazine	56617-70-0	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub>	1305	1318	[28]		-
279	1080	0.800	2,5-Dimethyl-3-isoamylpyrazine	18433-98-2	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub>	1317	1319	[67]		-
280	1092	0.850	2,3-Dimethyl-5-isopentylpyrazine	18450-01-6	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub>	1325	1332	[68]		-
<b>Pyridines</b>										
281	186	1.090	Pyridine	110-86-1	C <sub>5</sub> H <sub>5</sub> N	729	726	[28]	[91]	Pungent, nauseating, warm, burnt, smoky, coffee-like
282	270	1.020	2-Methylpyridine	109-06-8	C <sub>6</sub> H <sub>7</sub> N	827	824	[63]	[91]	Roasted popcorn, coffee
283	360	0.950	2,6-Dimethylpyridine	108-48-5	C <sub>7</sub> H <sub>9</sub> N	892	887	[5]	[91]	Minty-tarry, pyridine, peppermint
284	390	0.980	2-Ethylpyridine	100-71-0	C <sub>7</sub> H <sub>9</sub> N	911	919	[31]	[91]	-
285	480	1.200	3-Ethylpyridine	536-78-7	C <sub>7</sub> H <sub>9</sub> N	963	963	[28]	[91]	Tobacco, caramel, burnt, coffee-like, toasted
286	498	1.700	3-Vinylpyridine	1121-55-7	C <sub>7</sub> H <sub>7</sub> N	973	972	[5]		-
287	600	2.130	2-Acetylpyridine	1122-62-9	C <sub>7</sub> H <sub>7</sub> NO	1032	1045	[28]	[91]	Popcorn, bready, tobacco, cracker-like, roasted barley

288	786	2.450	Methyl 3-pyridinecarboxylate	93-60-7	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	1141	1137	[5]	[91]	Nauseating, sweet-herbaceous, mildly tobacco-like, fresh, caramel	[114, 116]
289	888	0.920	2-Pentylpyridine	2294-76-0	C <sub>10</sub> H <sub>15</sub> N	1201	1205	[69]		Tallowy-like	[116]
<b>Pyrroles</b>											
290	180	0.910	1-Methylpyrrole	96-54-8	C <sub>5</sub> H <sub>7</sub> N	720	731	[28]	[91]	Smokey-tarry, sweet, woody-herbaceous, animal, coffee	[109, 114]
291	204	5.870	Pyrrole	109-97-7	C <sub>4</sub> H <sub>5</sub> N	763	768	[28]	[91]	Warm, slightly pungent, hay-like herbaceous, sweet, green, toasted	[109, 114, 116, 129]
292	252	0.920	1-Ethylpyrrole	617-92-5	C <sub>6</sub> H <sub>9</sub> N	814	818	[63]	[91]	-	
293	330	1.100	2,5-Dimethylpyrrole	625-84-3	C <sub>6</sub> H <sub>9</sub> N	870	867	[28]	[91]	-	
294	426	0.970	2-Ethyl-4-methylpyrrole	69687-77-0	C <sub>7</sub> H <sub>11</sub> N	932	938	[70]	[98]	-	
295	474	2.390	1-Acetylpyrrole	609-41-6	C <sub>6</sub> H <sub>7</sub> NO	960	957	[71]	[91]	-	
296	528	0.920	3-Ethyl-2,4-dimethylpyrrole	517-22-6	C <sub>8</sub> H <sub>13</sub> N	990	988	[28]	[91]	-	
297	552	2.590	1-Methyl-2-formylpyrrole	1192-58-1	C <sub>6</sub> H <sub>7</sub> NO	1005	1010	[5]	[91]	Cracker-popcorn, burnt	[129, 130]
298	630	2.020	1-Ethyl-2-formylpyrrole	2167-14-8	C <sub>7</sub> H <sub>9</sub> NO	1049	1067	[70]	[91]	-	
299	672	2.070	2-Acetyl-1-methylpyrrole	932-16-1	C <sub>7</sub> H <sub>9</sub> NO	1074	1096	[31]	[91]	-	
300	672	2.850	2-Acetylpyrrole	1072-83-9	C <sub>6</sub> H <sub>7</sub> NO	1074	1098	[28]	[91]	Bread, walnut, licorice, cracker, popcorn-like	[109, 116, 130]
<b>Sulfur compounds</b>											
301	180	0.710	Dimethyl disulfide	624-92-0	C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>	719	719	[3]	[91]	Onion	[114, 116]
302	294	1.550	Methylthio-2-propanone	14109-72-9	C <sub>4</sub> H <sub>8</sub> OS	845	863	[72]		Melon	[116]
303	354	1.440	2-Furylmethylsulfide	13129-38-9	C <sub>5</sub> H <sub>6</sub> OS	888	894	[73]	[91]	Garlic-like	[130]
304	390	1.870	2-Furfurylthiol	98-02-2	C <sub>5</sub> H <sub>6</sub> OS	911	918	[63]	[91]	Coffee-like, caramellic-burnt, sweet, roasty, sulfury	[114, 118, 121, 128, 129]
305	390	2.060	3-(Methylthio)propanal (Methional)	3268-49-3	C <sub>6</sub> H <sub>8</sub> OS	912	912	[4]	[91]	Onion, meat-like, bouillon-like, soup-like, cooked potato-like	[114, 116, 117, 123, 128]
306	444	1.420	1-(Methylthio)-2-butanone	13678-58-5	C <sub>5</sub> H <sub>10</sub> OS	942	-	-	[91]	Mushroom, garlic	[116, 130]
307	486	1.190	Dimethyl trisulfide	3658-80-8	C <sub>2</sub> H <sub>6</sub> S <sub>3</sub>	966	969	[4]	[91]	Fresh onion, cabbage-like, brothy, sulfury, pungent	[98, 114, 116, 128]
308	510	3.580	3-Mercapto-3-methyl-1-butanol	34300-94-2	C <sub>5</sub> H <sub>12</sub> OS	981	-		[91]	Sweet, soup-like, cooked meat, spicy, smoke-roast, meaty, chicken	[98, 124, 130]
309	546	1.520	2-Furfuryl methyl sulfide	1438-91-1	C <sub>6</sub> H <sub>8</sub> OS	1001	995	[74]	[91]	Coffee-like, onion, garlic, burnt, sulfury, cooked cabbage	[98, 109, 116, 130]
310	582	1.540	3-Mercapto-3-methylbutyl formate	50746-10-6	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> S	1022	1020	[75]	[91]	Sweaty, fruity, black currant-like, catty, orange flowers, roasty	[118, 121, 124, 128, 130]
311	732	1.230	3-Mercapto-3-methylbutyl acetate	50746-09-3	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> S	1108	-	[76]	[112]	-	
312	906	1.950	Furfuryl methyl disulfide	57500-00-2	C <sub>6</sub> H <sub>8</sub> OS <sub>2</sub>	1212	1226	[29]	[91]	Fresh white bread crust	[130]
<b>Terpenic compounds</b>											
<i>Monoterpenes</i>											
313	426	0.440	α-Pinene	80-56-8	C <sub>10</sub> H <sub>16</sub>	931	932	[3]	[99]	Pine, turpentine-like	[116]
314	498	0.490	β-Pinene	127-91-3	C <sub>10</sub> H <sub>16</sub>	973	982	[77]	[99]	Turpentine, dry, woody, resinous	[116]
315	522	0.470	2,6-Dimethyl-2,6-octadiene (isomer)	2792-39-4	C <sub>10</sub> H <sub>18</sub>	986	990	[78]		-	
316	528	0.540	β-Myrcene	123-35-3	C <sub>10</sub> H <sub>16</sub>	990	988	[1]	[91]	Sweet, balsamic, plastic, sweet-balsamic-resinous gum	[114, 116]
317	552	0.470	2,6-Dimethyl-2,6-octadiene (isomer)	2792-39-4	C <sub>10</sub> H <sub>18</sub>	1004	990	[78]		-	
318	552	0.560	α-Phellandrene	99-83-2	C <sub>10</sub> H <sub>16</sub>	1004	1007	[77]	[113]	Fresh, citrus, peppery, discrete mint, minty, herbaceous	[116]
319	570	0.560	α-Terpinene	99-86-5	C <sub>10</sub> H <sub>16</sub>	1014	1016	[2]	[99]	Woody, terpene, lemon	[116]
320	582	0.670	p-Cymene	99-87-6	C <sub>10</sub> H <sub>14</sub>	1021	1026	[79]	[91]	Carrot-like, kerosene-like	[114, 116]
321	594	0.550	Limonene	138-86-3	C <sub>10</sub> H <sub>16</sub>	1028	1031	[46]	[91]	Citrusy, lemon-like, fresh, sweet	[130]
322	612	0.590	β-Ocimene (isomer)	13877-91-3	C <sub>10</sub> H <sub>16</sub>	1038	1042	[77]	[97]	Warm herbaceous	[116]
323	630	0.610	β-Ocimene (isomer)	13877-91-3	C <sub>10</sub> H <sub>16</sub>	1049	1042	[77]	[97]	Warm herbaceous	[116]
324	648	0.600	γ-Terpinene	99-85-4	C <sub>10</sub> H <sub>16</sub>	1059	1062	[80]	[99]	Lemon	[116]
325	696	0.610	α-Terpinolene	586-62-9	C <sub>10</sub> H <sub>16</sub>	1087	1093	[77]		Sweet, pine	[116]
326	702	0.940	p-Cymenene	1195-32-0	C <sub>10</sub> H <sub>12</sub>	1090	1095	[81]	[91]	Citrusy-lemon-like, gassy	[114]
327	786	0.790	Cosmene	460-01-5	C <sub>10</sub> H <sub>14</sub>	1140	1134	[82]		-	
328	798	0.670	Allo-ocimene	673-84-7	C <sub>10</sub> H <sub>16</sub>	1147	1144	[80]		-	
<i>Monoterpenoids</i>											
329	672	0.970	Linalool oxide (isomer)	1365-19-1	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	1073	1078	[83]	[91]	Sweet, woody, floral, woody-earthly undertone, pungent	[114, 116]
330	702	0.970	Linalool oxide (isomer)	1365-19-1	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	1090	1078	[83]	[91]	Sweet, woody, floral, woody-earthly undertone, pungent	[114, 116]
331	720	1.220	Linalool	78-70-6	C <sub>10</sub> H <sub>18</sub> O	1101	1101	[2]	[91]	Floral-woody, faintly citrusy note, floral, sweet-fruity	[114-116, 118, 124, 125]
332	876	1.430	α-Terpineol	98-55-5	C <sub>10</sub> H <sub>18</sub> O	1194	1206	[80]	[91]	Floral, lilac	[130]
333	888	1.200	Safranal	116-26-7	C <sub>10</sub> H <sub>14</sub> O	1201	1201	[5]		Saffron-like	[116]
334	918	1.050	p-Menth-1-en-9-al	29548-14-9	C <sub>10</sub> H <sub>16</sub> O	1219	1219	[80]		-	
<i>Sesquiterpenes</i>											
335	1152	0.560	α-Cubebene	17699-14-8	C <sub>15</sub> H <sub>24</sub>	1364	1366	[84]		-	
336	1170	0.560	α-Copaene	3856-25-5	C <sub>15</sub> H <sub>24</sub>	1376	1375	[84]	[28]	-	
337	1212	0.610	Longifolene	475-20-7	C <sub>15</sub> H <sub>24</sub>	1405	1395	[84]		-	
338	1236	0.620	β-Caryophyllene	87-44-5	C <sub>15</sub> H <sub>24</sub>	1421	1417	[84]		Cloves, turpentine	[116]
339	1296	0.650	α-Humulene	6753-98-6	C <sub>15</sub> H <sub>24</sub>	1455	1450	[84]		-	
340	1356	0.660	α-Muurolene	31983-22-9	C <sub>15</sub> H <sub>24</sub>	1505	1490	[84]		-	
341	1386	0.660	δ-Cadinene	483-76-1	C <sub>15</sub> H <sub>24</sub>	1525	1525	[84]	[28]	-	
<b>Norisoprenoids</b>											
342	1020	0.710	Vitispirane (C <sub>13</sub> )	65416-59-3	C <sub>13</sub> H <sub>20</sub> O	1279	1289	[3]		-	
343	1098	0.850	Theaspirane (C <sub>13</sub> )	36431-72-8	C <sub>13</sub> H <sub>22</sub> O	1329	1315	[85]		Fruity, woody, sweetish	[116]

344	1134	0.980	1,2-Dihydro-1,1,6-trimethylnaphthalene (TDN) (C <sub>13</sub> )	30364-38-6	C <sub>13</sub> H <sub>16</sub>	1353	1363	[3]		-	
345	1182	1.070	β-Damascenone (C <sub>13</sub> )	23726-93-4	C <sub>13</sub> H <sub>18</sub> O	1385	1395	[3]	[91]	Tea-like, fruity, honey-like, fruity, sweet-fruity	[118, 121, 124-127, 130]
346	1248	1.000	α-Ionone (C <sub>13</sub> )	127-41-3	C <sub>13</sub> H <sub>20</sub> O	1430	1439	[11]		Warm, woody, berry characteristic violet-like	[116]
347	1290	0.960	Geranyl acetone (C <sub>13</sub> )	689-67-8	C <sub>13</sub> H <sub>22</sub> O	1459	1463	[3]		Green and rosy floral, fresh-floral, sweet-rosy, slightly green	[116]
<b>Thiazoles</b>											
348	180	1.470	Thiazole	288-47-1	C <sub>3</sub> H <sub>5</sub> NS	720	730	[63]	[91]	Green, sweet, nutty, tomato, toasted	[109, 116]
349	252	1.150	2-Methylthiazole	3581-87-1	C <sub>4</sub> H <sub>5</sub> NS	814	815	[63]	[91]	-	
350	264	1.350	4-Methylthiazole	693-95-8	C <sub>4</sub> H <sub>5</sub> NS	823	823	[28]	[91]	Nutty, green, roasted	[116, 129]
351	294	1.330	5-Methylthiazole	3581-89-3	C <sub>4</sub> H <sub>5</sub> NS	844	846	[86]	[91]	-	
352	360	1.040	2,4-Dimethylthiazole	541-58-2	C <sub>5</sub> H <sub>7</sub> NS	892	892	[86]	[91]	Salty, sulfury, burnt, rubber	[98]
353	408	1.080	2,5-Dimethylthiazole	4175-66-0	C <sub>5</sub> H <sub>7</sub> NS	921	934	[72]	[91]	-	
354	432	1.270	4,5-Dimethylthiazole	3581-91-7	C <sub>5</sub> H <sub>7</sub> NS	935	947	[63]	[91]	Roasted nutty, boiled poultry	[116]
355	462	1.320	5-Ethylthiazole	17626-73-2	C <sub>5</sub> H <sub>7</sub> NS	952	955	[63]	[91]	-	
356	498	0.970	2-Ethyl-4-methylthiazole	15679-12-6	C <sub>6</sub> H <sub>9</sub> NS	973	-	-	[91]	Nutty, green	[116]
357	540	1.220	4-Propylthiazole	41981-60-6	C <sub>6</sub> H <sub>9</sub> NS	997	-	-		-	
358	564	1.030	5-Ethyl-2-methylthiazole	19961-52-5	C <sub>6</sub> H <sub>9</sub> NS	1011	1015	[86]	[91]	Rubber-like	[126]
359	576	0.870	2-Isopropyl-4-methylthiazole	15679-13-7	C <sub>7</sub> H <sub>11</sub> NS	1018	-	-		Green, vegetable, nutty, rooty, earthy	[116]
360	576	1.150	5-Ethyl-4-methylthiazole	31883-01-9	C <sub>6</sub> H <sub>9</sub> NS	1018	1039	[86]	[91]	Nutty, green, earthy	[130]
361	576	2.690	2-Acetylthiazole	24295-03-2	C <sub>5</sub> H <sub>5</sub> NOS	1019	1036	[63]	[91]	Green onion, herbal, grassy	[116]
362	660	0.880	4-Ethyl-2,5-dimethylthiazole	32272-57-4	C <sub>7</sub> H <sub>11</sub> NS	1066	1066	[86]	[91]	-	
363	678	0.940	5-Ethyl-2,4-dimethylthiazole	38205-61-7	C <sub>7</sub> H <sub>11</sub> NS	1076	1078	[86]	[91]	Earthy, roasty	[118]
364	738	1.990	2-Acetyl-4-methylthiazole	7533-07-5	C <sub>6</sub> H <sub>7</sub> NOS	1112	1128	[70]	[91]	-	
365	756	2.220	2-Propanoyl-thiazole	43039-98-1	C <sub>6</sub> H <sub>7</sub> NOS	1123	1119	[39]		-	
366	930	2.900	Benzothiazole	95-16-9	C <sub>7</sub> H <sub>5</sub> NS	1227	1231	[2]	[91]	Delicate, persistent, rose-like	[116]
<b>Tiophene compounds</b>											
367	126	0.650	Thiophene	110-02-1	C <sub>4</sub> H <sub>4</sub> S	637	626	[49]	[91]	-	
368	204	0.730	2-Methylthiophene	554-14-3	C <sub>5</sub> H <sub>6</sub> S	756	771	[63]	[91]	Onion, sulfury	[130]
369	216	0.770	3-Methylthiophene	616-44-4	C <sub>5</sub> H <sub>6</sub> S	774	783	[63]	[91]	-	
370	324	0.780	2-Ethylthiophene	872-55-9	C <sub>6</sub> H <sub>6</sub> S	866	872	[63]	[95, 97]	-	
371	330	0.740	2,5-Dimethylthiophene	638-02-8	C <sub>6</sub> H <sub>6</sub> S	870	877	[63]	[98]	-	
372	342	0.800	2,4-Dimethylthiophene	638-00-6	C <sub>6</sub> H <sub>6</sub> S	879	882	[63]		-	
373	354	0.840	2,3-Dimethylthiophene	632-16-6	C <sub>6</sub> H <sub>6</sub> S	888	898	[63]	[98]	-	
374	378	1.300	2-Vinylthiophene	1918-82-7	C <sub>6</sub> H <sub>6</sub> S	904	915	[63]	[98]	-	
375	414	1.660	3-Methoxythiophene	17573-92-1	C <sub>5</sub> H <sub>6</sub> OS	925	-	-		-	
376	456	2.670	3-Thiophanone	1003-04-9	C <sub>4</sub> H <sub>4</sub> OS	950	942	[87]	[91]	Garlic meaty, green vegetable, buttery	[116]
377	492	0.790	2-Isopropylthiophene	4095-22-1	C <sub>7</sub> H <sub>10</sub> S	969	976	[88]		-	
378	510	0.780	2,3,4-Trimethylthiophene	1795-04-6	C <sub>7</sub> H <sub>10</sub> S	980	993	[89]		-	
379	522	1.890	Dihydro-2-methyl-3(2H)-thiophenone	13679-85-1	C <sub>5</sub> H <sub>6</sub> OS	987	995	[63]	[91]	-	
380	528	3.660	3-Thiophenecarboxaldehyde	498-62-4	C <sub>5</sub> H <sub>4</sub> OS	992	1003	[49]		-	
381	540	2.880	Dihydro-2(3H)-thiophenone	1003-10-7	C <sub>4</sub> H <sub>6</sub> OS	998	-	-	[91]	-	
382	546	3.670	2-Thiophenecarboxaldehyde	98-03-3	C <sub>5</sub> H <sub>4</sub> OS	1002	1004	[90]	[91]	Coffee	[109]
383	690	2.550	3-Methyl-2-thiophenecarboxaldehyde	5834-16-2	C <sub>6</sub> H <sub>6</sub> OS	1084	1105	[66]	[91]	-	
384	690	3.220	3-Acetylthiophene	1468-83-3	C <sub>6</sub> H <sub>6</sub> OS	1085	-	-	[91]	-	
385	702	3.180	2-Acetylthiophene	88-15-3	C <sub>6</sub> H <sub>6</sub> OS	1092	1112	[63]	[91]	-	
386	708	0.830	2,5-Diethylthiophene	5069-23-8	C <sub>8</sub> H <sub>12</sub> S	1094	-	-		-	
387	738	2.260	Methyl-2-thiophene carboxylate	5380-42-7	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub> S	1112	-	-	[91]	-	
388	750	2.680	5-Methyl-2-thiophenecarboxaldehyde	13679-70-4	C <sub>6</sub> H <sub>6</sub> OS	1120	1124	[39]	[91]	-	
389	822	0.770	2-Pentylthiophene	4861-58-9	C <sub>9</sub> H <sub>14</sub> S	1161	1165	[63]		-	
390	864	2.390	2-Propionylthiophene	13679-75-9	C <sub>7</sub> H <sub>8</sub> OS	1187	1181	[90]	[91]	-	

<sup>a</sup> Retention times for first (<sup>1</sup>*t<sub>R</sub>*) and second (<sup>2</sup>*t<sub>R</sub>*) dimension in seconds.

<sup>b</sup> RI<sub>Calc</sub>: Retention Index obtained through the modulated chromatogram.

<sup>c</sup> RI<sub>Lit</sub>: Retention Index reported in the literature for 5% phenyl polysilphenylene-siloxane GC column or equivalents [1-90].

<sup>d</sup> Compound already identified in roasted coffee beans and/or brews [28, 91-113].

<sup>e</sup> Aroma descriptors [98, 109, 114-130].



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