

Table S1. Compounds identified using retention indices (RI) measured in the study and those reported in the literature, as well as using confirmation with reference compounds.

Compound	RI (measured) ^a	RI (literature) ^b
<i>Acetates</i>		
Ethyl acetate	891	888
2-Methylpropyl acetate*	1017	1012
3-methyl-1-butyl acetate*	1124	1123
Ethyl phenylacetate	1799	1783
2-phenylethyl acetate	1832	1813
<i>Esters</i>		
Ethyl butanoate	1041	1036
Ethyl 3-methylbutanoate*	1072	1068
Ethyl hexanoate*	1235	1233
Ethyl lactate ((L)-ethyl 2-hydroxypropanoate)	1349	1349
Ethyl octanoate*	1436	1435
Ethyl 3-hydroxybutyrate	1528	1532
Ethyl nonanoate	1538	1532
Ethyl 2-hydroxy-4-methylpentanoate	1550	1547
Isoamyl lactate (Isopentyl 2-hydroxypropanoate)	1577	1580
Ethyl 2-furoate	1630	1618
Methyl benzoate	1634	1640
Ethyl decanoate*	1642	1639
Diethyl succinate	1684	1681
Ethyl butyl succinate	1803	1820
Ethyl dodecanoate	1851	1843
Ethyl 3-methylbutyl succinate	1914	1901
<i>Aldehydes</i>		
3-methyl butanal*	922	918
Benzaldehyde*	1533	1528
4-methylbenzaldehyde	1663	1655
Dodecanal	1717	1711
<i>Alcohols</i>		
2-methyl-1-propanol	1107	1092
Butanol*	1157	1142
4-methyl-2-pentanol	1175	1168
3-methyl-1-butanol*	1217	1209
Hexanol*	1360	1355
cis-3-Hexen-1-ol*	1390	1382
2-Nonanol	1524	1521
Octanol*/octyl formate	1568	1553
3-(methylthio)-1-propanol	1737	1734
Phenylethyl alcohol*	1938	1907
<i>Volatile acids</i>		
Acetic acid*	1454	1449
2-methyl propanoic acid	1576	1570
Butanoic acid*	1640	1624
3-methyl butanoic acid	1681	1666
Hexanoic acid*	1860	1846

Octanoic acid*	2075	2060
Nonanoic acid*	2177	2170
Decanoic acid*	2267	2276
<i>Ketones</i>		
Butyrolactone	1647	1647
Acetophenone*	1666	1647
β -damascenone*	1841	1823
<i>Others</i>		
Toluene	1046	1042
1-(1-ethoxyethoxy)pentane	1096	1098
N-(3-Methylbutyl)acetamide	1883	1890

* Identified with external standard; ^a Kovats retention indices calculated using n-alkanes C7-C21; ^b Retention indices from the National Institute of Standards and Technology database (www.nist.gov);