

**Table S1.** Area of volatile compounds identified by HS-SPME/ GC×GC -ToFMS in white and red wines in contact with chitosan-genipin films during 2 and 8 months.

<sup>1</sup> t <sub>R</sub> <sup>a</sup> (s)	<sup>2</sup> t <sub>R</sub> <sup>a</sup> (s)	Volatile compound	Formula	CAS Number <sup>b</sup>	RI <sub>cal</sub> <sup>c</sup>	RI <sub>lit.</sub> <sup>d</sup>	MSI level <sup>e</sup>	logP <sup>f</sup>	Area (x10 <sup>5</sup> ) and RSD (%)			
									White wine		Red wine	
									2 months	8 months	2 months	8 months
		<b>Fatty Acids</b>										
		<i>Short chain fatty acids</i>										
95	3.176	Ethanoic acid (Acetic acid) # ♦	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	64-19-7	619	600	1	-0.28	518.02 <sup>g</sup> (6) <sup>h</sup>	962.62 (15)	1072.86 (10)	900.07 (4)
135	4.216	Propionic acid (Propanoic acid) #	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	79-09-4	716	707	1	0.25	–	–	16.21 (30)	–
175	4.632	Butyric acid (Butanoic acid) ♦	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	107-92-6	806	808	2	0.78	6.09 (7)	–	4.34 (44)	-
		<i>Medium chain fatty acids</i>							-			
360	3.864	Hexanoic acid (Caproic acid) # ♦	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	142-62-1	1015	1017	1	1.92	270.64 (18)	316.64 (18)	92.00 (32)	92.45 (17)
525	2.704	Octanoic acid (Caprylic acid) ♦	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	124-07-2	1203	1210	2	2.90	608.01 (17)	538.68 (10)	103.13 (22)	80.49 (22)
690	2.056	Decanoic acid (Caprinic acid) ♦	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	334-48-5	1372	1380	2	4.09	150.39 (38)	50.32 (32)	12.86 (6)	–
		<i>Long chain fatty acids</i>										
805	2.200	Dodecanoic acid (Lauric acid) #	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	143-07-7	1568	1568	1	5.03	15.39 (24)	–	–	–
940	1.912	Tetradecanoic acid (Myristic acid) # ♦	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	544-63-8	1765	1768	1	6.09	15.75 (52)	–	12.90 (34)	5.77 (5)
1070	1.488	Hexadecanoic acid (Palmitic acid) # ♦	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	57-10-3	1984	1985	1	7.15	35.10 (50)	–	30.94 (36)	–
		<i>Branched chain fatty acids</i>										
155	3.856	2-Methylpropanoic acid (Isobutyric acid) #	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	79-31-2	762	767	1	0.59	–	–	15.75 (9)	10.92 (3)
215	4.160	3-Methylbutanoic acid (Isovaleric acid) # ♦	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	503-74-2	855	861	1	1.13	8.24 (16)	–	18.92 (26)	27.73 (29)
225	3.896	2-Methylbutanoic acid (2-Methylbutyric acid) ♦	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	116-53-0	867	875	2	1.13	6.81 (11)	–	13.19 (21)	–
		<b>Ketones</b>										
		<i>Aliphatic ketones</i>										
115	0.632	Pentane-2,3-dione	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	600-14-6	660	658	2	-0.80	–	–	–	1.61 (5)
130	1.224	3-Hydroxy-butan-2-one (Acetoin) ♦	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	513-86-0	697	711	2	-0.43	14.50 (25)	5.46 (39)	–	1.14 (25)
140	0.712	Pent-3-en-2-one	C <sub>5</sub> H <sub>8</sub> O	3102-33-8 (E)	719	729	2	0.56	–	–	3.36 (55)	2.96 (14)
170	0.600	3-Ethoxy-butan-2-one (m/z: 73,45) ♦	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	–	790	–	3	<1	4.01 (9)	1.93 (7)	–	1.42 (4)
250	0.632	Heptan-2-one	C <sub>7</sub> H <sub>14</sub> O	110-43-0	895	889	2	1.97	2.37 (15)	0.21 (18)	–	–

260	0.688	4-Ethoxy-2-pentanone	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	33330-50-6	906	900	3	0.73	–	–	–	0.57
340	0.600	Octan-3-one#	C <sub>8</sub> H <sub>16</sub> O	106-68-3	985	985	1	2.30	1.32 (16)	–	–	–
335	0.736	6-Methyl-hept-5-en-2-one (Sulcatone) ♦	C <sub>8</sub> H <sub>14</sub> O	110-93-0	988	985	2	2.37	17.12 (16)	6.27 (14)	3.77 (19)	–
435	0.640	Nonan-2-one♦	C <sub>9</sub> H <sub>18</sub> O	821-55-6	1090	1100	2	3.03	12.17 (15)	2.42 (18)	–	0.85 (14)
455	1.112	Octane-2,5-dione	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	3214-41-3	1119	1088	2	0.79	1.27 (10)	–	–	–
520	0.680	Decan-2-one	C <sub>10</sub> H <sub>20</sub> O	693-54-9	1195	1190	2	3.56	0.53 (38)	0.83 (8)	–	–
600	0.648	Undecan-3-one	C <sub>11</sub> H <sub>22</sub> O	2216-87-7	1289	1283	2	4.09	1.21 (25)	–	–	–
605	0.672	Undecan-2-one	C <sub>11</sub> H <sub>22</sub> O	112-12-9	1295	1291	2	4.09	4.58 (12)	0.84 (44)	–	–
		<b>Aromatic ketones</b>										
415	1.304	1-Phenyl- ethanone (Acetophenone)# ♦	C <sub>8</sub> H <sub>8</sub> O	98-86-2	1074	1069	1	1.66	2.81 (21)	1.40 (23)	1.47 (10)	0.82 (6)
		<b>Volatile phenols</b>										
430	2.504	2-Methoxy-phenol (Guaiacol)#	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	90-05-1	1092	1090	1	1.19	0.29 (13)	0.44 (20)	–	–
600	1.664	4-Ethyl-2-methoxy-phenol (4-Ethylguaiacol)	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	2785-89-9	1284	1288	2	2.18	0.10 (27)	0.06 (45)	–	–
625	2.560	2-Methoxy-4-vinylphenol (p-Vinylguaiacol)	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	7786-61-0	1322	1327	2	1.93	6.66 (17)	0.59 (17)	–	–
780	0.704	2,6-bis(1,1-dimethylethyl)-4-methyl-phenol (BHT) ♦	C <sub>15</sub> H <sub>24</sub> O	128-37-0	1525	1514	2	5.32	4.44 (23)	1.30 (12)	–	2.43 (7)
780	1.488	2,4-bis(1,1-dimethylethyl)-phenol♦	C <sub>14</sub> H <sub>22</sub> O	96-76-4	1526	1512	2	4.86	43.55 (26)	22.18 (35)	6.15 (15)	1.31 (10)
		<b>Acetate esters</b>										
		<b>Saturated linear aliphatic acetate esters</b>										
75	0.456	Methyl ethanoate (Methyl acetate) ♦	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	79-20-9	566	559	2	0.18	8.02 (6)	1.89 (36)	2.49 (19)	8.22 (13)
125	0.520	n-Propyl ethanoate (n-Propyl acetate) ♦	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	109-60-4	684	712	2	1.24	45.95 (22)	15.14 (30)	18.86 (24)	7.97 (26)
190	0.560	Butyl ethanoate (Butyl acetate) ♦	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	123-86-4	819	812	2	1.77	13.39 (16)	3.31 (6)	13.96 (8)	4.94 (17)
270	0576	Pentyl ethanoate (Amyl acetate)	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	628-63-7	916	915	2	2.30	12.46 (7)	2.12 (55)		–
360	0.640	Hexyl ethanoate (Hexyl acetate)# ♦	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	142-92-7	1006	1014	1	2.83	268.62 (7)	95.94 (2)	51.48 (8)	–
455	0.592	Heptyl ethanoate (Heptyl acetate)	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	112-06-1	1118	1118	2	3.37	–	–	3.61 (18)	25.65 (4)
		<b>Unsaturated linear acetate esters</b>										
270	0.680	Pent-2-enyl ethanoate (Pent-2-enyl acetate)	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	42125-10-0(Z)	916	909	2	2.05	1.54 (3)	0.45 (25)	–	–
355	0.672	Hex-3-enyl ethanoate (Hex-3-enyl acetate)	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	3681-71-8	1006	1007	2	2.41	69.23 (6)	19.88 (13)	–	–
		<b>Branched acetate esters</b>										
160	0.520	2-Methylpropyl ethanoate (Isobutyl acetate) ♦	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	110-19-0	766	767	2	1.59	99.42 (4)	36.14 (6)	84.78 (12)	38.17 (4)
235	0.704	1-Methoxy-2-propyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	108-65-6	876	797	2	0.26	–	–	–	3.60 (12)
235		2-Methylbutyl ethanoate (2-Methylbutyl acetate)	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	624-41-9	879	885	2	2.12	7.44 (29)	6.81 (58)		

240	0.544	3-Methylbutyl ethanoate (Isoamyl acetate) ♦	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	123-92-2	882	876	2	2.12	598.11 (7)	316.36 (27)	455.05 (7)	124.16 (41)
330	0.600	4-Methyl-2-pentyl ethanoate (4-Methyl-2-pentyl acetate) ♦	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	108-84-9	980	—	3	2.47	52.38 (9)	11.49 (3)	3.88 (12)	1.90 (7)
880	1.016	Methyl dihydrojasmonate ♦	C <sub>13</sub> H <sub>22</sub> O <sub>3</sub>	24851-98-7	1671	1615	2	2.50	0.69 (31)	0.23 (46)	1.83 (29)	—
		<i>Aromatic acetate esters</i>										
580	1.064	2-Phenylethyl ethanoate (2-Phenylethyl acetate) ♦	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	103-45-7	1260	1256	2	2.30	214.74 (7)	91.26 (2)	54.99 (8)	35.58 (16)
		<i>Miscellaneous esters</i>										
		<i>Esters derived from butyric acid</i>										
300	0.536	2-Methylpropyl butanoate (Isobutyl butyrate)	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	539-90-2	949	961	2	2.65	—	—	1.37 (29)	0.51 (12)
365	0.520	3-Methylpropyl butanoate (Isoamyl butyrate) ♦	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	106-27-4	1017	1019	2	2.18	5.22 (46)	5.61 (11)	11.51 (14)	4.67 (13)
		<i>Esters derived from hexanoic acid</i>										
280	0.600	Methyl hexanoate (Methyl caproate) ♦	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	106-70-7	927	934	2	2.30	10.17 (8)	5.80 (19)	11.43 (7)	4.14 (7)
440	0.560	Propyl hexanoate (Propyl caproate) ♦	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	626-77-7	1101	1093	2	3.37	4.62 (17)	4.45 (44)	3.41 (17)	0.93 (23)
490	0.536	2-Methylpropyl hexanoate (Isobutyl caproate) ♦	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	105-79-3	1160	1148	2	3.71	4.00 (17)	3.54 (14)	4.44 (15)	2.27 (16)
575	0.552	3-Methylbutyl hexanoate (Isoamyl caproate) ♦	C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>	2198-61-0	1259	1250	2	4.24	42.63 (15)	24.84 (14)	139.13 (19)	8.72 (20)
		<i>Esters derived from octanoic acid</i>										
465	0.600	Methyl octanoate (Methyl caprylate) ♦	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	111-11-5	1130	1126	2	3.37	29.52 (16)	23.20 (10)	20.60 (17)	9.51 (17)
610	0.560	Propyl octanoate (Propyl caprylate) ♦	C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>	624-13-5	1301	1296	2	3.70	8.30 (5)	—	3.03 (16)	—
650	0.552	2-Methylpropyl octanoate (Isobutyl caprylate) ♦	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	5461-06-3	1351	1348	2	4.78	6.21 (10)	4.86 (16)	5.04 (18)	—
730	0.552	3-Methylbutyl octanoate (Isoamyl caprylate) ♦	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	2035-99-6	1456	1444	2	5.31	76.11 (15)	34.09 (17)	34.96 (23)	8.17 (22)
		<i>Esters derived from decanoic acid</i>										
635	0.600	Methyl decanoate (Methyl caprinate) ♦	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	110-42-9	1332	1326	2	4.43	5.22 (14)	1.85 (14)	3.15 (18)	0.46 (4)
755	0.616	Propyl decanoate (Propyl caprinate)	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	30673-60-0	1488	1481	2	5.49	2.79 (23)	—	—	—
870	0.568	3-Methylbutyldecanoate (Isoamyl decanoate) ♦	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	2306-91-4	1655	1651	2	6.37	17.85 (23)	8.04 (27)	8.07 (27)	—
		<i>Esters derived from dodecanoic acid</i>										
780	0.648	Methyl dodecanoate (Methyl laurate)	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	111-82-0	1326	1326	2	5.49	—	—	0.71 (23)	—
855	0.560	1-Methylethyl dodecanoate (Isopropyl laurate) ♦	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	10233-13-3	1632	1627	2	6.37	3.54 (20)	78.90 (9)	8.71 (66)	—
		<i>Esters derived from lactic acid</i>										
145	1.328	Methyl 2-hydroxypropanoate (Methyl lactate)	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>	547-64-8	732	748	2	-0.72	—	—	—	0.77 (9)
275	1.122	Propyl 2-hydroxypropanoate (Propyl lactate)	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	616-09-1	922	897	2	0.34	—	—	3.31 (15)	—
325	1.016	Butyl 2-hydroxy-propanoate (Butyl lactate)	C <sub>7</sub> H <sub>14</sub> O <sub>3</sub>	138-22-7	975	997	2	0.88	—	—	—	3.11 (20)
410	1.080	3-Methylbutyl 2-hydroxypropanoate (Isoamyl lactate) ♦	C <sub>8</sub> H <sub>16</sub> O <sub>3</sub>	19329-89-6	1068	1082	2	1.22	7.17 (2)	25.27 (9)	85.31 (21)	68.67 (7)

		<b>Other esters</b>										
170	0.568	3-Methylbutyl methanoate (Isoamyl formate)	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	110-45-2	780	792	2	1.71	–	–	1.67 (28)	–
320	0.560	Pentyl propanoate (Amyl propionate)	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	624-54-4	972	969	2	2.83	8.48 (32)	13.09 <sup>d</sup>	20.63 (10)	–
975	0.568	Methylethyl tetradecanoate (Isopropyl myristate) ♦	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	110-27-0	1834	1824	2	7.43	14.45	1.74 (34)	5.81 (4)	1.90 (26)
1100	0.592	Methylethyl hexadecanoate (Isopropyl palmitate) ♦	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>	142-91-6	2037	1999	2	8.49	8.00 (25)	18.13 (16)	2.84 (11)	4.55 (18)
		<b>Other aromatic esters</b>										
530	1.192	Methyl 2-hydroxybenzoate (Methyl salicylate) ♦	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	119-36-8	1207	1190	2	2.43	1.03	3.99 (9)	16.53 (9)	12.75 (14)
720	0.960	2-Phenylethyl butanoate (2-Phenylethyl butyrate)	C <sub>12</sub> H <sub>16</sub> O <sub>2</sub>	103-52-6	1439	1442	2	3.36	0.43 (25)	–	–	–
885	0.936	Hexyl 2-hydroxybenzoate (n-Hexyl salicylate) ♦	C <sub>13</sub> H <sub>18</sub> O <sub>3</sub>	6259-76-3	1678	1682	2	4.89	0.76 (17)	–	0.79 (32)	–
		<b>Ethyl esters</b>										
		<b>Ethyl esters of short chain fatty acids (C2-C5)</b>										
95	0.456	Ethyl ethanoate (Ethyl acetate)# ♦	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	141-78-6	613	613	1	0.73	488.42 (11)	455.23 (32)	632.21 (14)	349.56 (61)
125	0.496	Ethyl propanoate (Ethyl proprionate)# ♦	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	105-37-3	684	688	1	1.24	43.45 (23)	41.20 (10)	71.32 (40)	30.55 (7)
180	0.536	Ethyl butanoate (Ethyl butyrate)# ♦	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	105-54-4	807	800	1	1.77	250.41 (2)	151.04 (14)	204.20 (4)	103.33 (3)
260	0.552	Ethyl pentanoate (Ethyl valerate) ♦	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	539-82-2	906	898	2	2.12	4.11 (2)	5.62 (9)	9.64 (35)	4.33 (10)
		<b>Ethyl esters of medium chain fatty acids (C6-C10)</b>										
350	0.576	Ethyl hexanoate (Ethyl caproate)# ♦	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	123-66-0	1001	1001	1	2.83	639.81 (26)	337.85 (10)	606.59 (10)	128.31 (35)
440	0.658	Ethyl heptanoate# ♦	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	106-30-9	1100	1104	1	3.37	13.58 (16)	8.50 (20)	33.22 (19)	15.77 (11)
530	0.576	Ethyl octanoate (Ethyl caprylate)# ♦	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	106-32-1	1207	1199	1	3.90	997.73 (38)	1061.51 (11)	192.61 (40)	218.70 (29)
610	0.576	Ethyl nonanoate (Ethyl pelargonate)# ♦	C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>	123-29-5	1301	1294	1	4.43	25.95 (10)	11.88 (4)	30.75 (18)	8.54 (27)
690	0.584	Ethyl decanoate (Ethyl caprinate)# ♦	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	110-38-3	1401	1394	1	4.96	971.04 (43)	254.20 (5)	301.95 (12)	82.80 (33)
		<b>Ethyl esters of long chain fatty acids (C11-C18)</b>										
760	0.624	Ethyl undecanoate	C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>	627-90-7	1494	1494	2	5.49	–	–	5.49 (21)	–
835	0.592	Ethyl dodecanoate (Ethyl laurate) ♦	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	106-33-2	1601	1593	2	6.02	353.37 (13)	78.90 (3)	119.44 (14)	15.94 (18)
965	0.600	Ethyl tetradecanoate (Ethyl myristate) ♦	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	124-06-1	1801	1793	2	7.09	15.20 (35)	15.52 (49)	8.75 (25)	3.72 (16)
1085	0.616	Ethyl hexadecanoate (Ethyl palmitate) ♦	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	628-97-7	2010	1994	2	8.15	7.28 (32)	51.72 (46)	9.68 (7)	8.50 (19)
		<b>Unsaturated ethyl esters</b>										
210	0.656	Ethyl but-2-enoate ♦	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	623-70-1 (E)	845	844	2	1.85	18.84 (5)	16.86 (1)	10.30 (9)	6.69 (2)
340	0.632	Ethyl hex-5-enoate	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	54653-25-7	990	975	2	2.44	–	–	18.88 (21)	10.29 (3)
360	0.632	Ethyl hex-3-enoate ♦	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	26553-46-8	1012	1006	2	2.24	–	2.34 (8)	12.78 (12)	–

390	0.640	Ethyl hex-2-enoate♦	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	27829-72-7	1045	1040	2	2.91	13.40 (13)	12.13 (5)	44.56 (10)	25.29 (6)
435	0.616	Ethyl hept-4-enoate	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	54340-70-4 (E)	1095	1090	2	3.04	–	–	–	2.72 (8)
520	0.632	Ethyl oct-7-enoate	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	35194-38-8	1195	1186	2	3.39	–		–	5.22 (20)
570	0.640	Ethyl oct-2-enoate ♦	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	7367-82-0	1254	1246	2	3.77	3.04 (9)	0.90 (10)	1.30 (22)	–
675	0.672	Ethyl dec-9-enoate	C <sub>12</sub> H <sub>22</sub> O <sub>2</sub>	67233-91-4	1389	1382	2	4.45	–	–	201.65 (32)	–
		<i>Ethyl esters of branched fatty acids</i>										
150	0.488	Ethyl 2-methylpropanoate (Ethyl isobutyrate) ♦	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	97-62-1	742	762	2	1.59	23.42 (8)	31.64 (5)	50.23 (10)	28.67 (14)
215	0.512	Ethyl 2-methylbutanoate (Ethyl 2-methylbutyrate)# ♦	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	7452-79-1	851	849	1	2.12	10.75 (37)	13.26 (5)	19.51 (38)	7.81 (36)
220	0.528	Ethyl 3-methylbutanoate (Ethyl isovalerate) ♦	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	108-64-5	857	856	2	2.12	28.23 (31)	33.53 (4)	30.45 (17)	22.79 (6)
315	0.568	Ethyl 4-methyl-pentanoate (Ethyl isocaproate)	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	25415-67-2	964	968	2	2.65	–	–	1.22	–
		<i>Ethyl esters of diprotic acids</i>										
165	0.632	Diethyl carbonate	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	105-58-8	778	785	2	1.21		–	1.41 (55)	1.41 (6)
420	1.000	Diethyl propanedioate (Diethyl malonate)	C <sub>7</sub> H <sub>12</sub> O <sub>4</sub>	105-53-3	1079	1069	2	0.70	–	–	–	0.73 (33)
450	1.048	Ethyl methyl butanedioate (Ethyl methyl succinate)	C <sub>7</sub> H <sub>12</sub> O <sub>4</sub>	627-73-6	1113	1120	2	0.73	–	–	6.65 (20)	8.04 (15)
515	0.936	Diethyl butanedioate (Diethyl succinate)# ♦	C <sub>8</sub> H <sub>14</sub> O <sub>4</sub>	123-25-1	1189	1182	1	1.26	132.24 (10)	210.93 (21)	354.05 (18)	599.14 (7)
555	1.944	Monoethyl butanedioate (Ethyl hydrogen succinate)# ♦	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>	1070-34-4	1243	1141	1	0.32	8.62 (60)	–	138.99 (55)	–
595	0.880	Ethyl-n-propyl butanedioate (Ethyl-n-propyl succinate) ♦	C <sub>9</sub> H <sub>16</sub> O <sub>4</sub>	–	1283	–	2	1.79	–	0.78 (22)	3.34 (17)	3.13 (20)
640	0.816	Ethyl butyl butanedioate (Ethyl butyl succinate) ♦	C <sub>10</sub> H <sub>20</sub> O <sub>4</sub>	–	1339	1350	2	2.32	–	1.41 (8)	11.18 (19)	13.23 (17)
715	0.816	Ethyl 3-methylbutyl butanedioate (Ethyl isoamyl succinate) ♦	C <sub>11</sub> H <sub>24</sub> O <sub>4</sub>	28024-16-0	1435	1429	2	2.67	6.44 (28)	17.57 (5)	74.35 (17)	79.95 (19)
		<i>Miscellaneous ethyl esters</i>										
190	1.184	Ethyl 2-hydroxypropanoate (Ethyl lactate) ♦	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	97-64-3	820	848	2	-0.19	132.53 (7)	275.97 (22)	227.21 (50)	–
265	1.136	Ethyl 2-hydroxybutanoate	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	52089-54-0	912	947	2	0.34	–	–	0.65 (14)	–
300	1.352	Ethyl 3-hydroxy-butanoate#	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	5405-41-4	949	947	2	-0.02	–	–	7.72 (15)	4.95 (15)
320	0.936	Ethyl 2-hydroxy-3-methylbutanoate	C <sub>7</sub> H <sub>14</sub> O <sub>3</sub>	2441-06-7	969	975	2	0.69	–	–	5.95 (19)	3.19 (8)
340	0.744	Ethyl 3-ethoxy-propanoate	C <sub>7</sub> H <sub>14</sub> O <sub>3</sub>	763-69-9	990	960	2	1.25	–	–	5.22 (14)	–
405	0.952	Ethyl 2-hydroxy-4-methyl-pentanoate (Ethyl leucate) ♦	C <sub>8</sub> H <sub>16</sub> O <sub>3</sub>	10348-47-7	1062	1060	2	1.22	3.14 (9)	7.77 (6)	46.97 (10)	28.59 (9)
420	2.040	Ethyl 4-hydroxybutanoate	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	–	1080	1039	2	0.43	36.72 (25)	9.93 (19)	–	50.11 (21)
795	0.920	Ethyl 3-hydroxytridecanoate	C <sub>15</sub> H <sub>30</sub> O <sub>3</sub>	107141-15-1	1553	1539	2	4.76	0.97 (28)	1.56 (3)	–	–
		<i>Aromatic ethyl esters</i>										
510	0.960	Ethyl benzoate ♦	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	93-89-0	1184	1179	2	2.73	1.11 (5)	1.55 (4)	7.03 (11)	4.88(14)
570	1.016	Ethyl 2-phenylethanoate (Ethyl 2-phenylacetate)# ♦	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	101-97-3	1254	1251	1	2.50	3.51 (6)	3.20 (2)	3.85 (15)	5.59 (18)

585	1.112	Ethyl 2-hydroxybenzoate (Ethyl salicylate)	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	118-61-6	1272	1267	2	2.77	–	–	1.96 (10)	–
650	1.008	Ethyl 3-phenylpropanoate (Ethyl dihydrocinnamate)	C <sub>11</sub> H <sub>14</sub> O <sub>2</sub>	2021-28-5	1351	1347	2	2.79	–	–	1.74 (10)	1.62 (29)
725	1.920	Ethyl 2-hydroxy-3-phenylpropanoate (Ethyl 2-hydroxy-dihydrocinnamate)	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	15399-05-0	1449	1456	2	1.52	–	–	2.71 (54)	
		<b>Alcohols</b>										
		<i>Saturated aliphatic primary alcohols</i>										
80	0.712	Propan-1-ol (Propyl alcohol) ♦	C <sub>3</sub> H <sub>8</sub> O	71-23-8	578	595	2	0.34	14.82 (19)	128.53	39.80 (53)	6.93 (12)
105	0.816	Butan-1-ol (Butyl alcohol) ♦	C <sub>4</sub> H <sub>10</sub> O	71-36-3	637	653	2	0.88	19.74 (35)	14.98 (30)	29.22 (84)	27.95 (5)
160	0.944	Pentan-1-ol (Amyl alcohol)# ♦	C <sub>5</sub> H <sub>12</sub> O	71-41-0	767	768	1	1.41	–	4.30 (16)	13.26 (59)	–
230	1.040	Hexan-1-ol (Hexyl alcohol)# ♦	C <sub>6</sub> H <sub>14</sub> O	111-27-3	870	870	1	2.03	221.64 (1)	159.10 (31)	354.27 (19)	564.51 (3)
330	0.928	Heptan-1-ol (Heptyl alcohol) ♦	C <sub>7</sub> H <sub>16</sub> O	111-70-6	979	969	2	2.47	8.90 (3)	14.31 (32)	89.40 (8)	80.39 (17)
410	1.000	Octan-1-ol (Capryl alcohol)# ♦	C <sub>8</sub> H <sub>18</sub> O	111-87-5	1068	1070	1	3.00	22.30 (11)	30.70 (7)	45.64 (90)	73.50 (17)
515	0.880	Nonan-1-ol (Nonyl alcohol) ♦	C <sub>9</sub> H <sub>20</sub> O	143-08-8	1189	1171	2	3.53	6.90 (7)	6.93 (16)	35.61 (3)	–
595	0.856	Decan-1-ol (Capric alcohol)# ♦	C <sub>10</sub> H <sub>22</sub> O	112-30-1	1283	1272	1	4.06	14.52 (16)	9.99 (16)	20.75 (4)	10.96 (19)
740	0.880	Dodecan-1-ol (Lauric alcohol)# ♦	C <sub>12</sub> H <sub>26</sub> O	112-53-8	1470	1473	1	5.13	9.64 (36)	0.88 (23)	7.16 (26)	–
		<i>Unsaturated aliphatic primary alcohols</i>										
80	1.024	Prop-2-en-1-ol	C <sub>3</sub> H <sub>6</sub> O	107-18-6	579	555	2	0.17	–	–	28.03 (77)	–
160	1.200	Pent-2-en-1-ol	C <sub>5</sub> H <sub>10</sub> O	1576-95-0 (Z) 1576-96-1 (E)	768	769	2	1.22	–	–	5.87 (12)	4.33 (6)
220	1.112	(E)-Hex-3-en-1-ol♦	C <sub>6</sub> H <sub>12</sub> O	928-97-2	858	856	2	1.61	23.67 (2)	19.74 (12)	12.15 (3)	4.70 (11)
225	1.168	(Z)-Hex-3-en-1-ol# ♦	C <sub>6</sub> H <sub>12</sub> O	929-96-1	861	864	1	1.61	1.98 (16)	–	5.95 (3)	2.63 (10)
230	1.296	Hex-2-en-1-ol	C <sub>6</sub> H <sub>12</sub> O	928-95-0 (E)	870	862	1	1.75	–	–	10.63 (9)	6.69 (6)
315	1.200	Hept-4-en-1-ol	C <sub>7</sub> H <sub>14</sub> O	20851-55-2 (E)	964	870	2	2.07	–	–	8.08 (5)	–
320	1.264	Hept-2-en-1-ol	C <sub>7</sub> H <sub>14</sub> O	33467-76-4 (E)	970	–	2	2.29	–	–	1.88 (25)	–
420	1.104	Oct-2-en-1-ol	C <sub>8</sub> H <sub>16</sub> O	18409-17- 1 (E) 26001-58-1 (Z)	1079	1069	2	2.82	–	–	8.15 (10)	5.79 (8)
575	1.056	Dec-4-en-1-ol	C <sub>10</sub> H <sub>20</sub> O	57074-37-0 (Z)	1260	1257	2	3.67	–	–	3.78 (1)	–
590	0.664	Dec-2-en-1-ol	C <sub>10</sub> H <sub>20</sub> O	18409-18-2 (E)	1277	1283	2	3.88	5.13 (20)	–	–	–
770	0.664	Tridec-2-en-1-ol♦	C <sub>13</sub> H <sub>26</sub> O	74962-98-4 (E)	1511	1585	2	5.47	3.31 (80)	–	1.69 (21)	–
		<i>Unsaturated branched primary alcohols</i>										
90	0.800	2-Methyl-propan-1 -ol (Isobutyl alcohol) ♦	C <sub>4</sub> H <sub>10</sub> O	78-83-1	602	600	2	0.69	161.37 (48)	167.16 (8)	283.92 (27)	260.18 (3)
145	0.864	3-Methyl-butan-1-ol (Isoamyl alcohol) ♦	C <sub>5</sub> H <sub>12</sub> O	123-51-3	731	737	1	1.22	676.30 (18)	1230.35 (13)	1088.40 (37)	1856.22 (21)
215	0.992	3-Methyl-pentan-1-ol ♦	C <sub>6</sub> H <sub>14</sub> O	589-35-5	852	854	2	1.75	49.59 (3)	33.86 (10)	62.58 (5)	30.44 (6)

365	1.016	3-Ethyl-4-methylpentan-1-ol ♦	C <sub>8</sub> H <sub>18</sub> O	38514-13-5	1018	1020	2	2.63	1.75 (10)	2.03 (35)	6.45 (4)	6.35 (4)
380	0.880	2-Ethyl-hexan-1-ol ♦	C <sub>8</sub> H <sub>18</sub> O	104-76-7	1034	1029	2	2.82	5.72 (6)	18.53 (15)	6.75 (2)	7.95 (3)
		<i>Saturated aliphatic non primary alcohols</i>										
120	0.712	Pentan-2-ol (Methylpropyl carbinol) ♦	C <sub>5</sub> H <sub>12</sub> O	6032-29-7	672	706	2	1.22	–	0.93 (16)	5.18 (48)	4.80 (5)
260	0.832	Heptan-2-ol (Amyl methyl carbinol) ♦	C <sub>7</sub> H <sub>16</sub> O	543-49-7	906	905	2	2.39	3.95 (5)	3.79 (21)	16.01 (6)	13.26 (7)
355	0.752	Octan-2-ol	C <sub>8</sub> H <sub>18</sub> O	5978-70-1	1006	997	2	2.82	–	–	4.19 (21)	2.33 (12)
445	0.784	Nonan-2-ol ♦	C <sub>9</sub> H <sub>20</sub> O	628-99-9	1107	1098	2	3.35	16.14 (20)	17.49 (8)	14.52 (6)	15.36 (11)
620	0.744	Undecan-2-ol#♦	C <sub>11</sub> H <sub>24</sub> O	1653-30-1	1313	1309	1	4.41	3.64 (22)	2.10 (27)	2.17 (8)	–
120	0.688	Pentan-3-ol (Diethyl carbinol) ♦	C <sub>5</sub> H <sub>12</sub> O	584-02-1	672	710	2	1.22	–	0.49 (20)	1.63 (77)	2.14 (7)
350	0.832	Octan-3-ol (Ethyl amyl carbinol)#	C <sub>8</sub> H <sub>18</sub> O	20296-29-1	1001	994	1	2.82	–	–	5.21 (7)	4.65 (10)
		<i>Unsaturated non primary alcohols</i>										
110	0.816	Pent-1-en-3-ol ♦	C <sub>5</sub> H <sub>10</sub> O	616-25-1	649	656	2	1.05	–	1.18 (18)	9.40	5.09 (1)
340	0.960	6-Methyl-hept-5-en-2-ol (Sulcatol)	C <sub>8</sub> H <sub>16</sub> O	1569-60-4	990	992	2	2.44	–	–	6.19 (13)	3.10 (8)
335	0.936	Oct-1-en-3-ol# ♦	C <sub>8</sub> H <sub>16</sub> O	3391-86-4	980	980	2	2.64	2.31 (29)	3.93 (13)	14.83 (2)	10.57 (15)
		<i>Miscellaneous alcohols</i>										
155	4.840	Propane-1,2-diol (Propylene Glycol)	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	57-55-6	764	792	2	-1.34	19.40 (71)	1.73 (3)	–	–
170	3.144	Butane-2,3-diol isomer 1 ♦	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	513-85-9	805	806	2	-0.99	305. (41)	377.02 (69)	369.90 (17)	–
175	3.608	Butane-2,3-diol isomer 2 ♦	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	513-85-9	817	806	2	-0.99	126.86 (60)	198.78 (82)	87.35 (141)	–
215	1.184	3-Ethoxy-propan-1-ol ♦	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	111-35-3	845	–	3	0.16	5.76 (13)	8.56 (25)	21.15 (46)	1.86 (30)
		<i>Aromatic alcohols</i>										
400	2.960	Phenylmethanol (Benzyl alcohol)# ♦	C <sub>7</sub> H <sub>8</sub> O	100-51-6	1059	1043	1	1.03	1.73 (8)	3.57 (27)	102.46 (32)	92.60 (12)
465	2.296	Phenylethanol (Phenylethyl alcohol)# ♦	C <sub>8</sub> H <sub>10</sub> O	60-12-8	1132	1116	1	1.36	498.71 (27)	725.93 (6)	461.01 (8)	1638.13 (5)
		<i>Aldehydes</i>										
		<i>Saturated aliphatic aldehydes</i>										
100	0.472	3-Methylbutanal (Isovaleraldehyde) ♦	C <sub>5</sub> H <sub>10</sub> O	590-86-3	625	638	2	1.25	1.91 (38)	6.57 (5)	–	2.82 (13)
175	0.584	Hexanal# ♦	C <sub>6</sub> H <sub>12</sub> O	66-25-1	801	788	1	1.78	-	2.04 (13)	–	2.66 (19)
260	0.640	Heptanal	C <sub>7</sub> H <sub>14</sub> O	111-71-7	906	905	2	2.50	2.61 (14)	0.79 (15)	–	–
350	0.704	Octanal	C <sub>8</sub> H <sub>16</sub> O	124-13-0	1001	1001	2	3.03	–	–	3.28 (11)	15.32 (4)
445	0.632	Nonanal ♦	C <sub>9</sub> H <sub>18</sub> O	124-19-6	1106	1106	2	3.56	30.48 (10)	12.63 (11)	20.62 (19)	16.76 (11)
535	0.632	Decanal ♦	C <sub>10</sub> H <sub>20</sub> O	112-31-2	1207	1208	2	3.76	0.56	12.63 (26)	–	17.81 (16)
620	0.632	Undecanal ♦	C <sub>11</sub> H <sub>22</sub> O	112-44-7	1313	1310	2	4.63	6.41 (33)	-	2.92 (17)	1.14 (18)

700	0.624	Dodecanal ♦	C <sub>12</sub> H <sub>24</sub> O	112-54-9	1415	1409	2	5.16	15.00 (33)	3.43 (14)	5.92 (15)	3.00 (24)
		<i>Unsaturated aliphatic aldehydes</i>										
100	0.624	But-2-en-1-al	C <sub>4</sub> H <sub>6</sub> O	4170-30-3	625	624	2	0.63	–	1.50 (18)	–	–
220	0.744	(E)-Hex-2-enal#	C <sub>6</sub> H <sub>10</sub> O	6728-26-3	857	856	1	1.58	–	–	–	2.37 (5)
		<i>Aromatic aldehydes</i>										
310	1.360	Phenylmethanal (Benzaldehyde)# ♦	C <sub>7</sub> H <sub>6</sub> O	100-52-7	959	962	1	1.48	8.68 (5)	89.91 (5)	487.36 (3)	525.36 (9)
390	1.480	Phenylethanal (Phenylacetaldehyde) ♦	C <sub>8</sub> H <sub>8</sub> O	122-78-1	1046	1049	2	1.78	3.77 (10)	8.00 (13)	6.26 (14)	8.73 (21)
550	1.200	3,5-Dimethyl-benzaldehyde	C <sub>9</sub> H <sub>10</sub> O	5779-95-3	1219	1169	2	2.56	–	–	–	1.86 (12)
		<b>Furans</b>										
110	0.416	Tetrahydro-furan	C <sub>4</sub> H <sub>8</sub> O	109-99-9	648	623	2	0.33	11.45 (13)	10.77 (72)	–	–
205	1.808	2-Furanylmethanal (Furfural)# ♦	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	98-01-1	840	830	1	0.73	17.31 (4)	89.10 (4)	–	48.28 (5)
240	3.816	2-Furanylmethanol (Furfuryl alcohol)#	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	98-00-0	867	866	1	0.20	44.61 (6)	50.95 (4)	–	–
275	1.536	1-(2-Furanyl)-ethanone (2-Acetylfuran)#	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	1192-62-7	917	910	1	0.52	2.40 (3)	3.22 (3)	–	–
325	1.504	5-Methylfuran-2-carbaldehyde (5-Methylfurfural)	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	620-02-0	965	962	2	1.19	0.61 (9)	–	–	–
325	1.536	Methyl furan-2-carboxylate (Methyl 2-furoate)	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	611-13-2	975	983	2	0.99	1.09 (8)	1.20 (7)	–	–
345	0.568	2-Pentyl-furan ♦	C <sub>9</sub> H <sub>14</sub> O	3777-69-3	990	992	2	3.96	0.58 (16)	0.32 (26)	1.14 (28)	0.73 (20)
350	1.112	Benzofuran ♦	C <sub>8</sub> H <sub>6</sub> O	271-89-6	995	1006	2	2.67	1.94 (17)	1.26 (4)	0.47 (14)	0.39 (22)
345	1.224	Furfuryl ethanoate (Furfuryl acetate)	C <sub>7</sub> H <sub>8</sub> O <sub>3</sub>	623-17-6	1051	1062	2	1.09	0.45 (4)	–	–	–
365	1.272	1-(2-Furanyl)-propan-1-one (2-Propionylfuran)	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	3194-15-8	1007	1008	2	1.05	0.71 (12)	0.68 (6)	–	–
405	1.224	Ethyl 2-furancarboxylate (Ethyl 2-furoate) ♦	C <sub>7</sub> H <sub>8</sub> O <sub>3</sub>	614-99-3	1051	1062	2	1.52	11.43 (11)	15.97 (1)	1.45 (5)	1.07 (14)
485	0.696	2-n-Heptylfuran	C <sub>11</sub> H <sub>18</sub> O	3777-71-7	1154	1194	2	5.03	0.35 (22)	1.83 (15)	–	–
		<b>Lactones</b>										
275	2.336	Dihydro-2(3H)-furanone (γ-Butyrolactone)# ♦	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	96-48-0	918	915	1	-0.64	17.47 (14)	32.32 (19)	44.15 (37)	43.44 (9)
610	1.144	5-Butyl-dihydro-4-methyl-2(3H)-furanone (cis-Whiskey lactone)	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	39212-23-2	1301	1310	2	1.81	2.64 (19)	2.20 (9)	–	–
630	1.288	cis-4-Methyl-5-butyl-dihydro-2(3H)-furanone (β-Methyl-γ-octalactone)	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	55013-32-6	1327	1340	2	1.81	2.31 (22)	2.03 (10)	–	–
670	1.272	5-Pentyl-dihydro-2(3H)-furanone (γ-Nonanoic lactone)	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	104-61-0	1377	1360	2	1.85	–	-	1.03 (19)	0.99 (7)
		<b>Acetals (7)</b>										
130	0.488	1,1-Diethoxy-ethane (Diethyl acetal) ♦	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	105-57-7	695	719	2	1.14	73.01 (5)	91.00 (13)	11.68 (68)	68.80 (6)



[illegible]

285	0.448	$\alpha$ -Pinene#	C <sub>10</sub> H <sub>16</sub>	80-56-8	932	934	1	4.37	0.26 (26)	–	–	–
340	0.520	$\beta$ -Pinene ♦	C <sub>10</sub> H <sub>16</sub>	127-91-3	990	980	2	4.37	0.99 (11)	–	3.01 (18)	1.23 (10)
375	0.520	Limonene isomer# ♦	C <sub>10</sub> H <sub>16</sub>	5989-54-8	1028	1031	1	4.45	40.63 (13)	1.94 (19)	4.88 (36)	1.24 (47)
395	0.536	$\beta$ -Ocimene	C <sub>10</sub> H <sub>16</sub>	3779-61-1	1051	1050	2	4.70	–	–	–	0.69 (18)
400	0.632	<i>m</i> -Cymene#	C <sub>10</sub> H <sub>16</sub>	535-77-3	1056	1033	1	4.02	–	–	1.28 (16)	–
425	0.560	$\alpha$ -Terpinolene	C <sub>10</sub> H <sub>16</sub>	586-62-9	1084	1090	2	4.67	–	–	1.60 (19)	–
		<i>Ester type</i>										
565	0.592	Terpinen- 4-yl acetate	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	4821-04-9	1248	1265	2	3.80	–	–	–	3.13 (15)
580	0.522	Linalyl acetate ♦	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	115-95-7	1265	1264	2	3.93	4.04 (16)	3.46 (18)	1.62 (23)	4.52 (19)
585	0.600	$\alpha$ -Terpinyl acetate#	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	80-26-2	1271	1329	1	3.67	–	–	3.11 (19)	7.39 (51)
605	0.560	Endobornyl acetate ♦	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	76-49-3	1295	1285	2	3.30*	–	3.45 (8)	1.15 (17)	4.14 (26)
		<i>Alcohols type (10)</i>										
410	0.792	Dihydromyrcenol ♦	C <sub>10</sub> H <sub>20</sub> O	18479-58-8	1068	1072	2	3.00	2.80 (15)	–	5.44 (8)	–
435	0.896	Linalool# ♦	C <sub>10</sub> H <sub>18</sub> O	78-70-6	1095	1105	1	3.28	22.25 (15)	28.89 (5)	105.70 (2)	109.26 (4)
450	0.968	Ho-trienol ♦	C <sub>10</sub> H <sub>16</sub> O	29957-43-5	1112	1110	2	2.49	1.31 (8)	1.46 (1)	1.48 (23)	–
495	1.088	endo-Borneol ♦	C <sub>10</sub> H <sub>18</sub> O	507-70-0	1166	1165	2	2.58	0.56 (51)	1.05 (3)	0.77 (41)	–
505	1.096	Limonen-4-ol	C <sub>10</sub> H <sub>16</sub> O	3419-02-1	1178	1181	2	2.74	–		2.68 (5)	–
515	0.808	Terpinen-4-ol	C <sub>10</sub> H <sub>18</sub> O	562-74-3	1189	1206	2	2.99	–		4.93 (13)	13.19 (11)
520	0.992	$\alpha$ -Terpineol# ♦	C <sub>10</sub> H <sub>18</sub> O	98-55-5	1195	1224	1	2.79	3.54 (21)	7.20 (31)	46.30 (16)	77.42 (12)
525	0.944	Nerol#	C <sub>10</sub> H <sub>18</sub> O	106-25-2	1231	1234	1	3.28	–	–	9.90 (16)	3.36 (26)
550	1.080	Citronellol ♦	C <sub>10</sub> H <sub>18</sub> O	106-22-9	1242	1245	2	3.38	3.51 (12)	–	19.89 (6)	16.05 (18)
570	1.176	Geraniol # ♦	C <sub>10</sub> H <sub>18</sub> O	106-24-1	1272	1265	1	3.28	–	3.09 (39)	20.61(10)	17.62 (15)
		<i>Aldehydes type (2)</i>										
420	0.480	Citral	C <sub>10</sub> H <sub>16</sub> O	106-26-3	1079		2	3.17	–	–	1.55 (16)	–
780	0.944	Lilial	C <sub>14</sub> H <sub>20</sub> O	80-54-6	1537	1528	2	4.07	0.82 (23)	0.72 (7)	–	–
		<i>Oxide type</i>										
345	0.552	Dehydroxylinalool oxide isomer	C <sub>10</sub> H <sub>18</sub> O	7392-19-0	995	971	2	3.13	–	–	–	1.46 (1)
360	0.568	Dehydroxylinalool oxide isomer	C <sub>10</sub> H <sub>18</sub> O	7392-19-0	1012	971	2	3.13	–	–	–	1.31 (7)
345	0.552	Linalool oxide isomer 1	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	60047-17-8	1078	1074	2	2.15	–	–	2.50 (20)	17.39 (9)
360	0.568	Linalool oxide isomer 2	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	60047-17-8	1095	1074	2	2.15	–	–	4.97 (19)	16.90 (11)

420	0.736	Rose oxide isomer 1	C <sub>10</sub> H <sub>18</sub> O	16409-43-1	1107	1115	2	3.13	–	–	2.37 (19)	3.03(3)
435	0.752	Rose oxide isomer 2	C <sub>10</sub> H <sub>18</sub> O	16409-43-1	1130	1128	2	3.13	–	–	0.93 (10)	–
445	0.608	Nerol oxide♦	C <sub>10</sub> H <sub>16</sub> O	1786-08-9	1154	1155	2	2.2/2.85/3 .36	1.15 (44)	2.71 (8)	2.30 (21)	4.55 (16)
<b>Sesquiterpenic compounds (3)</b>												
695	0.584	Longifolene	C <sub>15</sub> H <sub>24</sub>	(+)-475-20-7 (-)-16846-09-6	1408	1402	2	6.39	–	–	3.63 (8)	–
815	0.784	Nerolidol# ♦	C <sub>15</sub> H <sub>26</sub> O	7212-44-4	1573	1564	1	5.32	6.57 (25)	6.05 (24)	-	1.76 (24)
995	0.792	(E,E)Farnesol# ♦	C <sub>15</sub> H <sub>26</sub> O	106-28-5	1801	1792	1	5.31	13.04 (32)	4.02 (15)	4.44 (35)	2.92 (42)

#Compound confirmed by co-injection of chemical standards;

♦Volatile compound determined either white or red wines

\*Retention times for first (<sup>1</sup>t<sub>R</sub>) and second (<sup>2</sup>t<sub>R</sub>) dimensions in seconds;

<sup>b</sup>CAS Chemical Abstract Service;

<sup>c</sup>RI: Retention Index obtained through the modulated chromatogram;

<sup>d</sup>RI: Retention Index reported in the literature for HP-5 (Equity-5) column or equivalents [1–18]

<sup>e</sup>Level of metabolite identification according to Sumner *et al.* (2007). (1) Identified compounds; (2) Putatively annotated compounds; (3) Putatively characterized compound classes; (4) Unknown compounds

<sup>f</sup>Log P: Logarithm of the octanol water partition coefficient was estimated using the ACD/Labs Percepta Platform – PhysChem Module (<http://www.chemspider.com/>)

<sup>g</sup>Mean of three replicates; <sup>h</sup>Relative standard deviation, expressed in parenthesis; and <sup>i</sup>The compound was only detected in one replicate

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