

Apparatus and Methods

Table 1 and 2 show the detailed parameters and analytical conditions of each detection unit in the GC-IMS technique used in this study.

Table 1 GC-IMS parameter settings for each analysis unit

Unit	Setting	Parameter
GC	Column Type	FS-SE-54-CB-1 15m ID:0.53mm
	Column Temperature	60 °C
	Carrier Gas	N ₂
IMS	Detector Model	FlavourSpec®
	IMS Temperature	45 °C
	IMS Drift Gas	N ₂
Automatic Sampling System	Injection Method	Headspace Injection
	Incubation Time	20 min
	Incubation Temperature	80 °C
	Incubation Speed	500 rpm
	Needle Temperature	85 °C
	Injection Volume	500 µL

Table 2 GC-IMS analysis condition

Time	E1 (IMS Drift Gas)	E2 (GC Carrier Gas)	Run
00:00,000	150 mL·min ⁻¹	2 mL·min ⁻¹	Rec
02:00,000	150mL·min ⁻¹	2 mL·min ⁻¹	2min
10:00,000	150mL·min ⁻¹	20mL·min ⁻¹	-
20:00,000	150mL·min ⁻¹	150 mL·min ⁻¹	15min
35:00,000	150mL·min ⁻¹	150 mL·min ⁻¹	Stop

Methodological verification

In order to verify the feasibility of the GC-IMS analytical method used in this experiment, we used this analytical method to detect 12 ppb hexanone and collected the signal intensity, IMS drift time and GC retention time for 18 days continuously (average test once every 5 min, 5138 times in total). Fig. 1 shows the range of fluctuations (a) and the distribution of deviations (b) of the three for 18 consecutive days of testing. The signal intensity values fluctuate from 0.323 to 0.396 (mean value 0.351) with the RSD of 2.604%; the drift time fluctuates from 12.79 to 13.02 (mean value 12.94) with the RSD of 0.371%, and the retention time fluctuates from 16.65 to 17.10 (mean value 16.80) with the RSD of 0.595%. The RSD of all three was controlled within 3%, proving that the instrument is precise and reliable, the system is stable and the method is feasible.

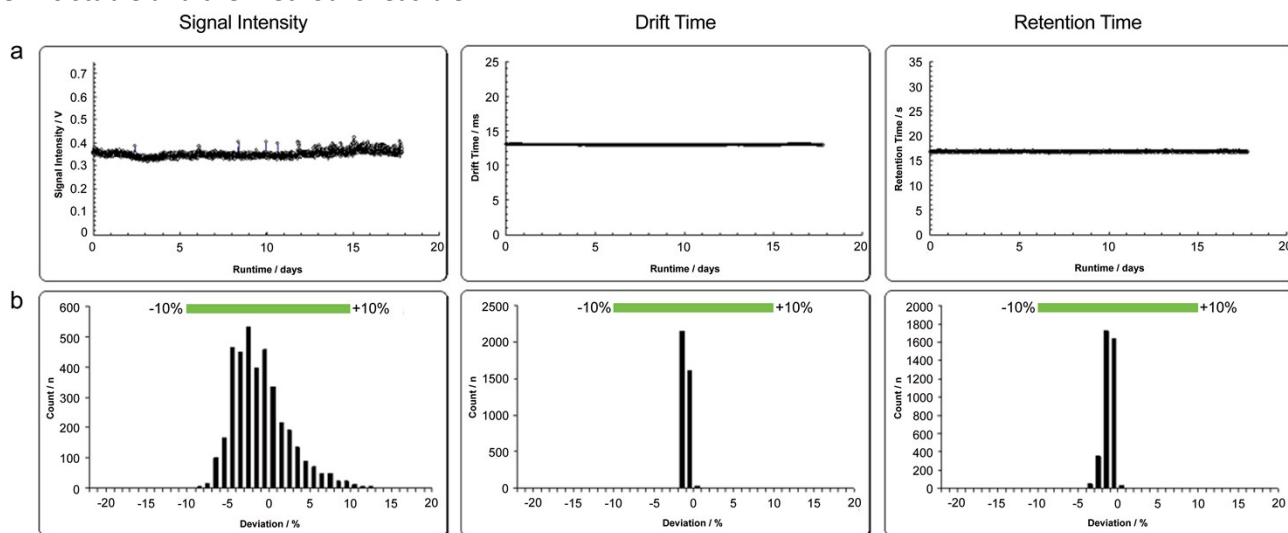


Figure 1 Validation of the feasibility of the GC-IMS analytical method

GC-IMS qualitative and quantitative

Fig. 2 shows the raw qualitative spectrum of the response signals in all samples. Tables 3-6 show the original GC-IMS data for the ten batches of samples (S1-H9) in this study. Due to the large amount of information, they were split into

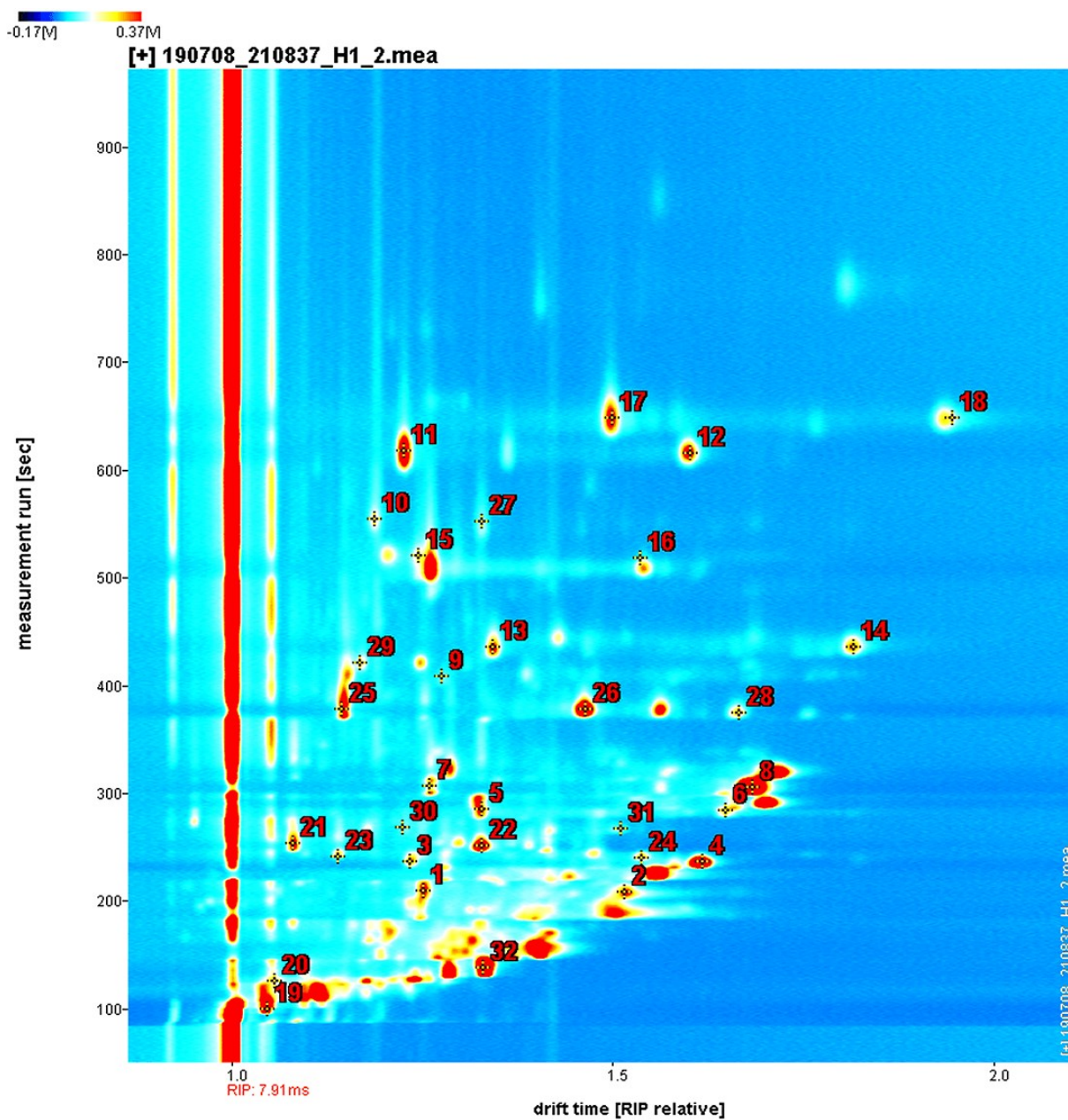


Figure 2 GC-IMS qualitative results for response signals
four tables.

Table 3 GC-IMS data for samples S1-H2

Compound	RI	Rt [sec]	Dt [RIPrel]	S1-1	S1-2	S1-3	H1-1	H1-2	H1-3	H2-1	H2-2	H2-3
1	531.3	114.854996	1.119	1318.416	1319.216	1292.43968	2050.628	2041.258	2005.02414	1970.925	1834.307	1864.56368
2	532.7	115.244995	1.094	2918.608	3159.896	2978.46696	1321.595	1254.015	1262.0489	1252.448	1182.769	1193.25633
3	540.3	117.39	1.147	817.183	1028.391	904.33126	599.74	694.992	634.41868	558.107	467.851	502.71942
4	670	161.06999	1.23	436.309	401.156	410.35785	86.964	77.387	80.53199	140.586	188.48	161.24234
5	728.4	190.31999	1.247	259.508	291.96	270.21932	268.028	293.794	275.29278	116.942	90.963	101.87345
6	696	172.37999	1.205	581.155	536.024	547.41771	872.138	905.06	870.82702	967.619	967.765	948.33816
7	705.5	177.45	1.156	219.058	194.409	202.59883	245.608	284.5	259.75292	495.742	644.744	558.83814
8	681.3	165.555	1.317	400.392	449.127	416.26431	547.23	579.16	551.9311	608.164	612.615	598.18171
1-pentanol monomer	763.2	211.575	1.252	583.163	628.846	593.88441	786.643	772.522	763.99085	453.206	389.442	412.89752
10	789.5	228.93	1.278	421.657	424.052	414.39741	333.016	327.55	323.67734	396.037	368.701	374.72162
1-hexanol monomer	871.8	287.81998	1.324	1390.224	1426.271	1380.08255	1134.59	1077.976	1084.15734	748.931	611.885	666.79984
12	910.5	323.895	1.285	693.621	714.74	690.09689	652.144	624.376	625.4948	423.218	397.547	402.17485
13	827.8	254.67	1.298	21.481	23.565	22.07254	140.136	160.887	147.50127	162.219	150.124	153.04807
14	650.2	153.465	1.407	876.763	887.386	864.43301	3130.513	2789.501	2900.80686	2550.488	2428.829	2439.86533
15	691.9	170.235	1.417	90.957	105.808	96.41485	625.95	585.735	593.72565	279.77	203.782	236.94048
Butyl acetate dimer	801.8	236.92499	1.615	1290.519	1328.783	1283.45798	1872.514	1826.165	1812.35271	991.65	916.94	935.2091
17	951.5	371.47498	1.331	145.525	161.778	150.57847	91.046	86.646	87.06908	49.052	52.658	49.8379
1-hexanol dimer	869.1	285.675	1.654	827.242	961.83	876.64528	681.714	680.978	667.71908	173.467	135.429	151.35904
19	874.7	290.16	1.703	1505.019	1523.959	1484.19922	1658.924	1620.21	1606.77566	525.683	470.668	488.21199
Ethyl valerate dimer	893.5	305.955	1.681	4067.579	4133.078	4018.32193	4270.235	4233.779	4166.96686	2276.376	2193.482	2190.23042
21	908.4	321.555	1.713	1703.275	1717.819	1676.33606	1983.138	2016.957	1960.04655	548.049	484.875	506.13276
22	1004.3	444.99	1.686	93.06	94.808	92.05532	93.85	76.379	83.41221	98.44	71.744	83.39016
1-octen-3-one	979.3	407.745	1.275	50.454	51.942	50.17404	72.69	77.308	73.49902	48.868	55.58	51.17952
24	968.5	393.31497	1.211	48.065	52.807	49.42728	29.455	32.402	30.30993	22.023	25.807	23.4367
25	941.6	359.38498	1.207	45.023	42.153	42.71624	29.563	24.358	26.42129	27.057	25.966	25.98127
26	1045.1	520.45496	1.205	571.686	592.066	570.23848	522.844	471.946	487.4471	371.536	316.369	337.07345
27	1063.6	558.675	1.187	465.488	498.343	472.27719	429.578	420.195	416.38877	362.35	311.716	330.29234
Methyl benzoate monomer	1095.1	630.435	1.226	3182.23	3123.3	3089.7097	2575.524	2412.75	2444.25426	2043.742	1722.691	1845.55217
Methyl benzoate dimer	1090.2	618.735	1.6	1754.633	1724.797	1704.9207	1459.13	1377.625	1390.00995	1039.233	876.373	938.64694

Compound	RI	Rt [sec]	Dt [RIPrel]	S1-1	S1-2	S1-3	H1-1	H1-2	H1-3	H2-1	H2-2	H2-3
Ethyl hexanoate monomer	1002.3	441.675	1.342	1067.61	1173.58	1098.1831	999.228	979.507	969.58015	266.702	264.218	260.1508
31	982.4	412.03497	1.386	79.846	87.747	82.12057	168.281	153.198	157.52471	139.34	116.561	125.39149
32	1027.5	486.525	1.261	65.514	67.84	65.34346	144.447	146.911	142.76542	71.021	48.281	58.45798
33	915.4	329.15997	1.327	307.319	338.998	316.69533	224.822	237.615	226.59413	155.85	124.076	137.16374
34	759.5	209.23499	1.298	166.911	189.59	174.68549	76.766	71.982	72.88652	109.516	126.116	115.45968
Ethyl hexanoate dimer	999.9	437.58	1.818	497.512	590.389	533.07149	780.261	863.387	805.38752	121.253	103.867	110.3088
36	690.8	169.65	1.18	971.511	1039.642	985.46497	588.73	546.523	556.27397	496.342	446.196	461.84362
37	807.4	240.62999	1.82	69.01	61.524	63.96166	41.55	36.751	38.36749	34.026	35.787	34.20837
38	1109.8	666.89996	1.26	91.975	118.1	102.93675	174.244	154.556	161.112	136.758	133.459	132.40633
39	1299	1377.87	1.213	1091.78	1017.213	1033.40657	910.364	830.312	852.93124	791.915	714.201	737.99684
40	861.4	279.63	0.951	92.419	75.062	82.06569	202.906	246.594	220.255	485.031	517.096	491.04223
41	1047.2	524.55	1.266	482.471	338.909	402.4762	2549.013	2621.572	2533.58665	2169.213	1897.091	1992.48896
phenylacetaldehyde dimer	1040.5	511.28998	1.541	40.782	36.802	38.01616	482.81	561.032	511.48258	425.663	316.975	363.89262
n-Nonanal monomer	1104.2	652.86	1.499	493.021	408.728	441.85701	1819.193	1769.389	1758.40518	1372.953	1182.982	1252.40815
n-Nonanal dimer	1103	649.74	1.937	82.095	85.866	82.30089	792.156	809.107	784.61887	545.425	412.89	469.57435
45	1004.5	445.37997	1.426	184.363	193.562	185.18325	366.331	332.933	342.63936	237.339	175.9	202.48711
46	827	254.08499	1.389	21.95	22.448	21.75502	127.067	136.881	129.33452	52.655	48.614	49.62181
47	902.9	315.705	1.349	31.568	34.029	32.14253	61.743	54.279	56.85078	81.635	67.123	72.89142
48	820.6	249.59999	1.414	41.169	59.894	49.52087	202.218	211.804	202.87078	238.338	230.849	229.90163
49	901.2	313.94998	1.446	18.61	20.704	19.26386	23.688	29.186	25.90826	60.217	53.721	55.82962
50	888	301.08	1.361	27.574	29.62	28.02506	24.526	27.431	25.45893	31.127	25.817	27.90256
ethanol	484.9	102.57	1.047	2006.49	2247.546	2084.47764	1600.169	1375.934	1458.29047	1498.05	1462.105	1450.47595
Furfurol monomer	829.7	256.035	1.08	115.841	116.828	114.00781	692.806	694.379	679.72065	717.221	692.489	690.7579
53	908	321.16498	1.575	49.892	48.202	48.06606	127.717	133.456	127.97477	108.869	97.12	100.93461
54	893.9	306.345	1.564	52.157	46.314	48.25079	131.847	142.493	134.4266	170.114	157.157	160.36279
55	814.3	245.31	1.475	107.337	106.89	104.97123	234.991	244.685	235.04124	281.772	235.613	253.51865
56	782.5	224.44499	1.446	88.232	78.041	81.47377	393.553	379.273	378.68474	438.32	389.68	405.72
57	781.4	223.665	1.415	156.329	177.978	163.81043	428.743	322.31	368.01597	308.563	300.709	298.54328
58	732.4	192.65999	1.312	57.581	54.727	55.03092	76.467	94.947	83.99286	76.667	68.747	71.25286
59	756.4	207.28499	1.449	54.904	47.542	50.19854	88.686	90.088	87.59926	85.822	89.815	86.06213

Compound	RI	Rt [sec]	Dt [RIPrel]	S1-1	S1-2	S1-3	H1-1	H1-2	H1-3	H2-1	H2-2	H2-3
60	783.9	225.42	1.522	79.31	81.616	78.85374	233.367	264.155	243.78578	199.132	162.609	177.25309
1-pentanol dimer	759.5	209.23499	1.52	385.902	412.883	391.40465	961.665	937.669	930.67366	256.247	199.455	223.29398
Acetic acid	574.9	127.725	1.061	736.002	728.691	717.69957	495.517	620.973	547.0801	668.369	749.978	694.99003
63	812.6	244.13998	1.282	46.064	46.762	45.48474	100.02	102.703	99.33427	115.905	110.008	110.69737
64	788.5	228.34499	1.557	455.112	452.426	444.69362	2502.984	2483.686	2443.4683	2551.354	2300.35	2377.33496
Z-3-hexen-1-ol dimer	845	267.15	1.507	17.731	16.571	16.80798	98.535	111.375	102.8559	71.64	61.702	65.33758
66	989.4	421.78497	1.247	210.507	216.283	209.1271	390.223	366.483	370.78594	267.742	221.288	239.6247
Ethyl lactate dimer	811.7	243.555	1.539	56.728	47.041	50.84681	264.773	282.41	268.11967	210.319	165.594	184.19737
Benzaldehyde dimer	961.2	383.75998	1.464	418.044	403.555	402.58351	1980.289	1957.305	1929.42106	2217.031	1923.821	2029.01748
Furfurol dimer	829.7	256.035	1.329	60.312	64.544	61.17944	1211.821	1265.742	1214.00587	1437.116	1335.238	1358.45346
70	1002.2	441.47998	1.467	98.675	100.556	97.62319	107.956	131.965	117.56129	111.102	178.048	141.6835
Phenylacetaldehyde monomer	1045.9	522.01495	1.24	279.986	260.25	264.71564	636.586	712.593	661.09771	974.388	1336.386	1132.27926
72	1092.3	623.61	1.363	187.874	234.09	206.76236	244.831	358.503	295.63366	650.663	990.355	804.09882
73	1103.1	649.935	1.529	132.973	98.161	113.25566	308.493	339.008	317.27549	427.199	535.77	471.85481
74	712.6	181.34999	1.081	134.823	141.335	135.31742	205.885	203.24	200.47125	130.68	102.392	114.20528
75	827.5	254.47499	1.272	23.14	19.397	20.84313	76.515	80.423	76.89962	79.877	75.294	76.03379
Ethyl lactate monomer	814.3	245.31	1.141	43.412	31.333	36.62505	196.366	192.642	190.61392	211.496	189.489	196.48265
77	845	267.15	1.184	291.532	302.733	291.18985	307.89	330.116	312.62294	315.938	419.129	360.18283
Butyl acetate monomer	805.9	239.655	1.239	819.702	784.524	786.07074	578.63	557.349	556.62971	451.851	509.179	470.9047
Ethyl valerate monomer	896.5	309.07498	1.26	785.457	780.512	767.32481	576.273	546.853	550.33174	708.289	644.062	662.65199
Benzaldehyde monomer	960.1	382.395	1.148	770.07	749.962	744.81568	1320.408	1251.23	1260.10262	1228.027	1090.994	1136.32029
81	982.1	411.645	1.45	32.706	27.771	29.63373	67.072	60.312	62.41816	98.291	159.704	126.41755
82	982.4	412.03497	1.476	29.741	29.233	28.89726	41.293	52.376	45.89781	69.267	71.538	68.99445
83	733.1	193.04999	1.335	45.988	57.245	50.58417	106.129	101.729	101.85042	89.555	90.097	88.02948
84	753.6	205.53	1.345	48.846	54.143	50.46461	45.55	49.451	46.55049	72.255	75.214	72.25981
85	876.9	291.91498	1.395	58.317	71.671	63.69412	40.291	41.258	39.95901	57.692	112.216	83.25492
86	958.6	380.44498	1.383	64.341	61.169	61.4999	76.699	92.895	83.10106	132.72	184.915	155.64115
87	961.7	384.34497	1.289	116.025	101.342	106.50983	154.603	157.398	152.88049	284.129	502.121	385.2625
88	1144.4	761.67	1.406	101.479	141.401	119.0112	169.112	177.676	169.92612	183.954	157.972	167.54374

Compound	RI	Rt [sec]	Dt [RIPrel]	S1-1	S1-2	S1-3	H1-1	H1-2	H1-3	H2-1	H2-2	H2-3
89	1144.5	762.06	1.539	56.887	55.094	54.87069	54.714	84.686	68.306	88.584	104.048	94.38968
90	1104.1	652.47	1.586	58.089	68.319	61.93992	112.885	137.455	122.6666	170.01	175.751	169.42289
E -2-octenal	1062.2	555.75	1.326	150.064	175.548	159.54988	318.986	332.21	319.08604	263.619	260.056	256.60075
92	1059.8	550.68	1.46	39.098	42.632	40.0477	71.992	75.421	72.23237	94.481	124.047	107.07872
93	1031.8	494.52	1.369	37.036	44.668	40.03496	57.724	74.539	64.80887	74.085	92.902	81.82363
E 2-heptenal	959.5	381.615	1.665	126.553	132.342	126.85855	367.077	402.685	377.18338	173.175	162.632	164.54543
95	961	383.56497	1.563	183.034	177.924	176.86942	850.778	920.61	867.98012	753.915	655.557	690.64128
96	739.7	196.95	0.956	217.862	226.157	217.56931	113.11	94.002	101.48488	235.197	188.008	207.37045
97	800	235.75499	1.586	55.025	64.014	58.32911	236.875	232.295	229.8933	216.873	200.394	204.46083
98	569.2	125.96999	1.174	290.936	350.658	314.38106	367.53	385.852	369.15718	359.692	324.296	335.15412
99	571.7	126.74999	1.214	101.523	89.146	93.42781	193.587	171.443	178.8647	178.685	165.674	168.73591
100	554.3	121.48499	1.196	102.855	123.185	110.7596	221.929	250.883	231.67788	180.49	184.087	178.64273
101	717.2	183.885	1.394	106.579	114.82	108.48551	343.233	323.503	326.70064	94.009	85.111	87.7688
6-methyl-5-hepten-2-one	992	425.49	1.17	142.953	118.239	127.98408	208.201	225.58	212.55269	200.981	189.286	191.23083
103	984.7	415.155	1.15	131.784	164.652	145.25364	594.95	602.068	586.53882	403.78	328.743	358.93627
104	787.3	227.56499	1.376	214.192	199.363	202.64195	226.31	266.112	241.28678	295.773	345.386	314.16791
105	729.8	191.09999	1.51	431.687	504.135	458.55278	2319.928	2297.283	2262.43339	237.25	199.509	214.01191
106	913	326.625	1.412	73.232	87.83	78.92038	94.135	53.648	72.41367	118.408	167.107	139.90235
107	898.4	311.025	1.387	40.075	58.657	48.37868	50.974	64.538	56.60088	103.03	181.384	139.36286
108	891.3	303.81	1.645	227.699	243.102	230.69249	262.949	246.607	249.68244	184.227	168.237	172.70736
Z-3-hexen-1-ol monomer	845.8	267.735	1.227	81.219	74.726	76.41305	97.529	104.362	98.92659	136.428	135.746	133.36526
110	868.1	284.895	1.228	50.869	44.992	46.97189	69.828	92.537	79.55885	99.623	115.416	105.36911
111	845.5	267.53998	1.418	43.72	58.257	49.96873	212.857	215.556	209.92237	221.831	189.213	201.41156
112	965.9	389.805	1.237	46.492	43.812	44.24896	70	64.331	65.82219	81.552	75.919	77.16079
113	415.4	86.579994	1.085	34.892	59.627	46.31431	68.369	134.877	99.59054	182.412	227.994	201.09894
114	636.4	148.39499	1.365	159.65	168.89	160.9846	622.213	539.357	569.1693	518.479	522.796	510.22475
Ethyl Acetate	597.4	134.94	1.331	1982.617	1885.113	1895.1877	3435.273	3088.139	3196.47188	2669.282	2659.614	2611.15904
116	582.9	130.26	1.286	658.406	628.5	630.58394	1494.148	1342.168	1389.79484	1735.63	1682.518	1674.89252
117	569.8	126.16499	1.243	294.628	301.181	291.94641	1014.041	1016.299	994.8666	1306.322	1236.934	1246.19544

Table 4 GC-IMS data for samples H3-H5

Compound	RI	Rt [sec]	Dt [RIPrel]	H3-1	H3-2	H3-3	H4-1	H4-2	H4-3	H5-1	H5-2	H5-3
1	531.3	114.854996	1.119	1663.638	1711.973	1654.04939	1697.309	1712.242	1670.67999	1936.699	1844.455	1852.76546
2	532.7	115.244995	1.094	1499.833	1560.269	1499.44998	1515.88	1397.149	1427.38421	1466.692	1433.014	1420.85594
3	540.3	117.39	1.147	521.391	640.833	569.48976	541.419	580.682	549.82949	537.847	604.805	559.89948
4	670	161.06999	1.23	232.628	209.044	216.41928	189.013	189.711	185.57476	245.269	224.254	230.06627
5	728.4	190.31999	1.247	53.895	51.371	51.58034	27.901	37.826	32.20623	44.732	39.012	41.03456
6	696	172.37999	1.205	1116.449	1102.149	1087.11302	1597.064	1570.901	1552.30285	1196.51	1150.285	1149.92955
7	705.5	177.45	1.156	848.846	986.054	899.101	808.219	860.824	817.83107	1105.769	1210.036	1134.74445
8	681.3	165.555	1.317	644.246	610.889	615.01615	1445.604	1388.299	1388.61247	720.755	722.502	707.19593
1-pentanol monomer	763.2	211.575	1.252	244.387	229.726	232.31537	200.131	206.316	199.15903	195.034	194.009	190.63107
10	789.5	228.93	1.278	305.575	282.083	287.95242	288.16	296.775	286.61815	253.992	245.031	244.52127
1-hexanol monomer	871.8	287.81998	1.324	500.808	476.783	479.01959	505.182	479.232	482.36286	460.714	450.868	446.67518
12	910.5	323.895	1.285	390.61	394.216	384.56474	408.446	407.643	399.88361	382.067	371	369.00283
13	827.8	254.67	1.298	189.07	185.816	183.69414	130.629	115.02	120.36801	132.326	129.424	128.2575
14	650.2	153.465	1.407	1546.534	1348.271	1418.45445	918.884	889.841	886.27525	955.2	899.329	908.71921
15	691.9	170.235	1.417	119.448	116.362	115.5469	70.958	63.294	65.78348	84.791	77.105	79.32904
Butyl acetate dimer	801.8	236.92499	1.615	1107.386	1039.135	1051.79529	1000.274	987.469	973.99407	1172.501	1144.664	1135.41085
17	951.5	371.47498	1.331	53.375	51.069	51.17756	46.026	48.176	46.15898	48.544	51.656	49.098
1-hexanol dimer	869.1	285.675	1.654	102.535	81.102	89.98213	85.603	89.352	85.72795	88.448	84.873	84.92729
19	874.7	290.16	1.703	573.215	493.119	522.50366	654.39	660.144	644.12166	680.515	694.865	673.9362
Ethyl valerate dimer	893.5	305.955	1.681	2559.814	2313.111	2387.73325	2716.428	2761.819	2684.34103	2862.844	2944.409	2845.55397
21	908.4	321.555	1.713	575.191	575.578	563.87681	760.379	840.32	784.34251	799.157	810.122	788.54671
22	1004.3	444.99	1.686	70.84	60.189	64.20421	48.703	60.95	53.72997	47.348	40.846	43.21506
1-octen-3-one	979.3	407.745	1.275	48.592	51.555	49.07203	50.438	47.072	47.7799	54.504	53.432	52.88864
24	968.5	393.31497	1.211	19.98	26.302	22.67818	27.818	24.853	25.80879	29.192	22.331	25.24627
25	941.6	359.38498	1.207	27.885	24.913	25.87102	23.784	23.454	23.14662	28.234	30.359	28.71057
26	1045.1	520.45496	1.205	279.609	239.099	254.16692	253.909	233.554	238.85687	223.15	236.834	225.39216
27	1063.6	558.675	1.187	307.119	285.156	290.21475	299.005	302.901	294.93394	260.843	238.427	244.6423
Methyl benzoate monomer	1095.1	630.435	1.226	1700.963	1546.432	1591.22355	1515.321	1433.268	1444.80861	1345.28	1370.751	1330.85519
Methyl benzoate dimer	1090.2	618.735	1.6	850.353	774	795.93297	682.855	614.918	635.90877	613.569	603.819	596.52012

Compound	RI	Rt [sec]	Dt [RIPrel]	H3-1	H3-2	H3-3	H4-1	H4-2	H4-3	H5-1	H5-2	H5-3
Ethyl hexanoate monomer	1002.3	441.675	1.342	254.055	232.041	238.18704	339.74	349.408	337.68252	275.669	289.474	276.92007
31	982.4	412.03497	1.386	114.582	104.143	107.17525	125.7	121.726	121.23874	127.47	114.468	118.54962
32	1027.5	486.525	1.261	44.89	39.863	41.52897	51.355	53.239	51.25106	34.534	35.974	34.54892
33	915.4	329.15997	1.327	138.363	121.453	127.30984	123.965	129.687	124.28948	150.749	142.071	143.4818
34	759.5	209.23499	1.298	132.98	131.295	129.49475	125.405	111.023	115.84972	117.957	133.709	123.31634
Ethyl hexanoate dimer	999.9	437.58	1.818	92.607	74.748	82.00395	137.04	151.171	141.22339	124.098	108.949	114.19303
36	690.8	169.65	1.18	393.087	331.401	354.99912	277.978	260.447	263.82825	320.623	336.996	322.23331
37	807.4	240.62999	1.82	37.658	46.876	41.42166	35.117	35.631	34.66652	34.413	32.364	32.72073
38	1109.8	666.89996	1.26	118.021	108.695	111.09084	118.35	100.178	107.07872	111.623	116.032	111.55095
39	1299	1377.87	1.213	656.455	650.691	640.50154	607.467	570.294	577.10289	609.519	588.818	587.18513
40	861.4	279.63	0.951	509.864	508.357	498.92829	486.781	466.23	466.97539	422.758	404.474	405.34368
41	1047.2	524.55	1.266	1408.492	1186.198	1271.3981	1100.719	1080.605	1068.84876	879.529	808.889	827.32482
phenylacetaldehyde dimer	1040.5	511.28998	1.541	167.992	137.024	149.45784	124.948	112.466	116.33286	74.704	68.388	70.11508
n-Nonanal monomer	1104.2	652.86	1.499	1149.028	1017.394	1061.54678	1216.922	1140.445	1155.10983	1164.955	1149.492	1134.07903
n-Nonanal dimer	1103	649.74	1.937	488.52	419.123	444.74507	555.541	519.77	526.90239	603.302	582.865	581.22183
45	1004.5	445.37997	1.426	151.4	111.505	128.82345	134.467	127.264	128.24819	114.325	107.306	108.59919
46	827	254.08499	1.389	49.604	43.31	45.52786	36.478	39.796	37.37426	40.104	35.872	37.22824
47	902.9	315.705	1.349	42.492	47.85	44.26758	47.428	48.992	47.2458	45.883	42.505	43.31012
48	820.6	249.59999	1.414	169.987	180.934	171.95129	161.937	155.317	155.45446	142.949	131.096	134.28205
49	901.2	313.94998	1.446	60.043	67.557	62.524	61.569	47.009	53.20322	62.092	67.25	63.37758
50	888	301.08	1.361	27.32	39.583	32.78247	30.105	28.653	28.79142	35.714	31.381	32.87655
ethanol	484.9	102.57	1.047	1402.357	1318.302	1333.12291	1238.105	1168.368	1179.17177	1163.88	1080.507	1099.74963
Furfurol monomer	829.7	256.035	1.08	696.73	674.297	671.80323	708.403	707.277	693.6832	647.681	631.834	626.96235
53	908	321.16498	1.575	115.642	110.547	110.83261	99.001	84.372	89.85277	87.988	89.447	86.94315
54	893.9	306.345	1.564	165.404	197.787	177.96359	213.853	224.993	215.03454	183.037	169.102	172.54811
55	814.3	245.31	1.475	199.671	200.014	195.84565	189.207	173.404	177.67939	151.263	137.376	141.43311
56	782.5	224.44499	1.446	376.742	384.605	373.06003	394.451	382.768	380.83731	374.207	361.567	360.52926
57	781.4	223.665	1.415	294.52	303.51	293.0347	317.99	291.535	298.66725	303.535	307.018	299.17097
58	732.4	192.65999	1.312	52.065	60.465	55.1397	77.749	94.646	84.47355	54.327	54.168	53.16255
59	756.4	207.28499	1.449	92.188	98.361	93.36901	81.171	93.542	85.60937	86.275	76.388	79.70487

Compound	RI	Rt [sec]	Dt [RIPrel]	H3-1	H3-2	H3-3	H4-1	H4-2	H4-3	H5-1	H5-2	H5-3
60	783.9	225.42	1.522	109.082	202.957	152.89911	188.134	226.16	203.00406	213.453	220.197	212.4885
1-pentanol dimer	759.5	209.23499	1.52	106.811	85.07	94.02169	75.459	70.228	71.38663	81.984	78.678	78.72438
Acetic acid	574.9	127.725	1.061	1169.494	1278.877	1199.70179	1232.04	1320.199	1250.59711	1373.149	1375.976	1347.07125
63	812.6	244.13998	1.282	111.134	112.891	109.77225	106.205	113.51	107.66035	109.773	94.716	100.19961
64	788.5	228.34499	1.557	2158.727	2226.554	2148.78769	2284.44	2277.585	2235.39225	2472.013	2384.392	2379.63845
Z-3-hexen-1-ol dimer	845	267.15	1.507	74.079	77.904	74.47167	75.103	87.271	79.56326	107.746	90.082	96.93572
66	989.4	421.78497	1.247	384.278	364.257	366.78215	452.714	431.934	433.47752	431.275	408.95	411.71025
Ethyl lactate dimer	811.7	243.555	1.539	149.934	173.508	158.48658	140.57	152.262	143.48768	142.378	128.456	132.70866
Benzaldehyde dimer	961.2	383.75998	1.464	1775.971	1666.286	1686.70593	1621.279	1596.315	1576.62106	1223.215	1141.524	1158.72211
Furfurol dimer	829.7	256.035	1.329	1447.66	1441.598	1415.73642	1788.951	1800.729	1758.9432	1425.735	1324.932	1347.82683
70	1002.2	441.47998	1.467	189.955	201.882	192.00013	320.448	347.822	327.4523	332.156	374.191	346.11003
Phenylacetaldehyde monomer	1045.9	522.01495	1.24	1122.174	1118.346	1097.8548	1124.718	1052.616	1066.89366	982.701	971.885	957.74714
72	1092.3	623.61	1.363	931.683	1019.963	956.30654	1034.304	1023.982	1008.56014	1155.487	1172.251	1140.59162
73	1103.1	649.935	1.529	573.066	586.284	568.0815	679.972	687.338	669.9819	820.796	821.913	804.92741
74	712.6	181.34999	1.081	75.059	87.798	79.79993	93.095	97.434	93.35921	92.026	98.529	93.37195
75	827.5	254.47499	1.272	90.037	96.822	91.56091	56.078	52.465	53.18607	68.049	68.214	66.76887
Ethyl lactate monomer	814.3	245.31	1.141	129.142	114.953	119.60655	108.463	112.485	108.26452	90.51	84.886	85.94404
77	845	267.15	1.184	430.831	521.496	466.64023	575.908	611.86	582.00632	656.423	714.28	671.64447
Butyl acetate monomer	805.9	239.655	1.239	530.619	554.789	531.84992	521.648	530.999	515.79703	597.154	626.654	599.66592
Ethyl valerate monomer	896.5	309.07498	1.26	608.929	574.611	579.9346	565.155	551.807	547.31138	516.316	498.407	497.21427
Benzaldehyde monomer	960.1	382.395	1.148	1027.668	956.961	972.46821	923.588	991.291	938.29071	838.563	822.278	813.81209
81	982.1	411.645	1.45	178.552	184.36	177.82688	246.338	257.757	247.00655	299.113	313.33	300.09707
82	982.4	412.03497	1.476	106.351	99.712	100.97087	136.187	146.594	138.56269	157.487	139.952	145.74511
83	733.1	193.04999	1.335	46.219	43.634	44.02797	64.369	98.097	79.60834	37.69	33.252	34.76158
84	753.6	205.53	1.345	104.352	89.343	94.91055	147.419	151.999	146.71482	109.129	85.86	95.54461
85	876.9	291.91498	1.395	136.84	147.517	139.33493	152.668	169.182	157.7065	218.51	275.393	242.01247
86	958.6	380.44498	1.383	210.205	216.724	209.19521	215.328	261.896	233.83976	309.159	323.42	309.96371
87	961.7	384.34497	1.289	505.449	562.973	523.52678	572.353	573.488	561.46209	674.741	686.126	666.82483
88	1144.4	761.67	1.406	217.713	195.896	202.66841	261.005	261.763	256.15632	311.021	301.838	300.30091

Compound	RI	Rt [sec]	Dt [RIPrel]	H3-1	H3-2	H3-3	H4-1	H4-2	H4-3	H5-1	H5-2	H5-3
89	1144.5	762.06	1.539	127.159	155.666	138.58425	181.476	205.552	189.64372	273.414	254.004	258.43482
90	1104.1	652.47	1.586	219.927	231.724	221.30899	244.266	231.524	233.1371	250.877	258.94	249.81033
E -2-octenal	1062.2	555.75	1.326	283.748	289.369	280.82733	340.803	330.253	328.81744	297.004	302.235	293.62711
92	1059.8	550.68	1.46	135.644	150.889	140.40117	187.253	196.353	187.96694	189.939	193.222	187.74889
93	1031.8	494.52	1.369	81.945	82.177	80.41978	93.78	99.572	94.74248	82.39	83.059	81.07001
E 2-heptenal	959.5	381.615	1.665	178.812	158.835	165.44703	194.609	217.241	201.8065	186.78	190.859	185.04311
95	961	383.56497	1.563	684.473	622.359	640.34768	673.742	680.8	663.72558	587.036	572.346	568.09718
96	739.7	196.95	0.956	192.74	169.835	177.66175	95.227	115.952	103.47771	121.71	145.627	130.99513
97	800	235.75499	1.586	177.302	207.626	188.61472	208.54	211.465	205.80245	247.096	223.674	230.6773
98	569.2	125.96999	1.174	268.231	244.84	251.40479	266.308	251.958	253.95034	270.032	272.307	265.74611
99	571.7	126.74999	1.214	139.159	137.528	135.57663	110.053	126.947	116.13	138.137	133.186	132.94827
100	554.3	121.48499	1.196	160.199	175.932	164.70419	143.473	160.37	148.88307	144.764	146.416	142.6782
101	717.2	183.885	1.394	75.145	40.836	56.83069	48.151	41.043	43.70506	39.783	43.374	40.74693
6-methyl-5-hepten-2-one	992	425.49	1.17	174.473	172.807	170.1672	165.182	170.841	164.65127	179.136	174.086	173.07878
103	984.7	415.155	1.15	258.102	250.363	249.14785	267.336	270.074	263.3309	198.83	188.934	190.00436
104	787.3	227.56499	1.376	435.788	600.637	507.84825	532.16	647.339	577.95451	629.461	642.635	623.32704
105	729.8	191.09999	1.51	159.758	133.56	143.72582	108.251	90.963	97.61486	96.118	139.644	115.52338
106	913	326.625	1.412	175.459	210.126	188.93665	230.367	265.671	243.05862	307.9	331.287	313.20163
107	898.4	311.025	1.387	172.795	229.364	197.05791	219.962	251.251	230.89437	296.179	303.154	293.67317
108	891.3	303.81	1.645	163.402	179.922	168.22876	179.789	174.682	173.69079	174.774	166.666	167.3056
Z-3-hexen-1-ol monomer	845.8	267.735	1.227	218.697	221.958	215.92095	238.255	245.963	237.26682	209.041	198.621	199.75438
110	868.1	284.895	1.228	166.54	192.049	175.70861	196.62	216.15	202.2573	205.022	190.282	193.69896
111	845.5	267.53998	1.418	206.611	210.621	204.44368	226.934	233.688	225.70478	212.898	188.357	196.61495
112	965.9	389.805	1.237	96.924	118.925	105.76601	112.92	111.953	110.18777	140.231	140.57	137.59249
113	415.4	86.579994	1.085	226.306	183.449	200.77995	209.244	165.553	183.65053	177.727	148.015	159.61358
114	636.4	148.39499	1.365	339.823	281.696	304.54431	295.015	259.162	271.54673	231.715	223.981	223.29104
Ethyl Acetate	597.4	134.94	1.331	2552.54	2353.77	2404.0919	3589.844	3288.508	3370.39248	2555.214	2372.39	2414.52596
116	582.9	130.26	1.286	1212.088	1076.091	1121.20771	1013.454	907.608	941.32038	869.442	811.734	823.77624
117	569.8	126.16499	1.243	714.902	684.311	685.61437	531.903	518.955	514.92042	480.615	471.071	466.32614

Table 5 GC-IMS data for samples H6-H8

Compound	RI	Rt [sec]	Dt [RIPrel]	H6-1	H6-2	H6-3	H7-1	H7-2	H7-3	H8-1	H8-2	H8-3
1	531.3	114.854996	1.119	1604.785	1824.376	1680.28889	2027.219	1579.697	1767.38884	1859.74	1461.201	1627.26109
2	532.7	115.244995	1.094	1393.818	1464.192	1400.4249	1328.951	1390.973	1332.76276	1472.823	1464.522	1439.29905
3	540.3	117.39	1.147	478.439	560.54	509.09971	482.48	465.361	464.44209	530.079	487.746	498.73425
4	670	161.06999	1.23	269.614	231.734	245.66052	224.841	244.139	229.8002	255.365	258.578	251.83207
5	728.4	190.31999	1.247	42.67	48.547	44.69633	81.197	77.219	77.62384	72.188	52.294	60.99618
6	696	172.37999	1.205	1099.177	1053.738	1054.92835	896.049	924.895	892.26256	1072.298	1078.734	1054.00568
7	705.5	177.45	1.156	1124.798	1201.471	1139.87181	1127.716	1038.3	1061.34784	1265.666	1235.707	1225.67277
8	681.3	165.555	1.317	564.73	527.916	535.39654	537.013	498.42	507.36217	698.528	612.158	642.23614
1-pentanol monomer	763.2	211.575	1.252	198.913	198.551	194.75736	235.734	233.155	229.75561	188.141	184.008	182.35301
10	789.5	228.93	1.278	221.859	236.108	224.40383	252.412	252.098	247.2099	269.966	243.54	251.61794
1-hexanol monomer	871.8	287.81998	1.324	540.509	547.582	533.16459	484.796	519.139	491.92815	529.68	476.558	493.05662
12	910.5	323.895	1.285	443.027	395.463	410.8601	384.389	409.93	389.21631	405.121	386.867	388.07412
13	827.8	254.67	1.298	117.545	104.07	108.59135	122.788	135.911	126.76251	134.106	133.757	131.25287
14	650.2	153.465	1.407	1055.93	877.464	947.36306	1040.676	1247.563	1121.23711	992.1	1018.428	985.15872
15	691.9	170.235	1.417	92.239	89.961	89.278	150.867	147.936	146.41347	105.789	98.313	100.00998
Butyl acetate dimer	801.8	236.92499	1.615	2049.569	1836.188	1904.02093	1581.759	1596.909	1557.54732	1846.447	1608.432	1692.89071
17	951.5	371.47498	1.331	79.056	65.143	70.65751	57.781	61.01	58.20759	65.467	62.587	62.74646
1-hexanol dimer	869.1	285.675	1.654	142.156	129.817	133.26677	107.639	123.007	113.01654	124.428	105.983	112.90139
19	874.7	290.16	1.703	1822.19	1583.021	1668.55339	1191.787	1327.368	1234.38595	1566.277	1201.005	1355.96818
Ethyl valerate dimer	893.5	305.955	1.681	4572.723	4326.878	4360.80449	3711.008	4012.082	3784.3141	4261.55	3766.42	3933.7053
21	908.4	321.555	1.713	2115.578	1852.772	1944.4915	1379.785	1523.369	1422.54546	1725.486	1327.831	1496.12533
22	1004.3	444.99	1.686	62.292	48.065	54.07493	51.469	49.391	49.4214	54.882	45.404	49.14014
1-octen-3-one	979.3	407.745	1.275	48.16	56.271	51.17119	63.097	74.399	67.37304	46.486	49.54	47.05274
24	968.5	393.31497	1.211	27.222	31.26	28.65618	30.705	24.951	27.27144	25.636	28.818	26.68246
25	941.6	359.38498	1.207	30.248	31.463	30.23839	33.925	33.607	33.09068	32.25	34.997	32.95103
26	1045.1	520.45496	1.205	215.198	206.637	206.69915	215.204	191.557	199.31289	227.639	187.062	203.20349
27	1063.6	558.675	1.187	264.094	258.036	255.8437	245.592	273.23	254.22278	258.163	237.424	242.83763
Methyl benzoate monomer	1095.1	630.435	1.226	1288.565	1318.14	1277.28545	1126.501	1150.735	1115.84564	1262.063	1100.386	1157.60001
Methyl benzoate dimer	1090.2	618.735	1.6	563.119	600.304	570.07727	469.161	439.677	445.33062	508.573	414.19	452.15387

Compound	RI	Rt [sec]	Dt [RIPrel]	H6-1	H6-2	H6-3	H7-1	H7-2	H7-3	H8-1	H8-2	H8-3
Ethyl hexanoate monomer	1002.3	441.675	1.342	773.153	669.26	706.78237	415.554	545.156	470.7479	570.367	438.504	494.34679
31	982.4	412.03497	1.386	144.316	130.433	134.62701	132.203	127.064	127.04083	126.014	121.221	121.14515
32	1027.5	486.525	1.261	51.447	43.675	46.60978	64.42	62.46	62.1712	42.825	41.173	41.15902
33	915.4	329.15997	1.327	136.916	157.42	144.22464	149.959	150.556	147.25235	137.861	144.583	138.39756
34	759.5	209.23499	1.298	128.713	127.245	125.41942	127.286	129.161	125.65903	121.193	123.467	119.8834
Ethyl hexanoate dimer	999.9	437.58	1.818	769.616	549.727	646.47807	252.101	436.324	337.32825	487.051	301.01	386.14989
36	690.8	169.65	1.18	405.908	390.124	390.05568	356.282	438.751	389.56617	390.813	404.316	389.61321
37	807.4	240.62999	1.82	34.727	33.233	33.3004	34.778	30.6	32.03522	30.714	30.889	30.18547
38	1109.8	666.89996	1.26	109.269	101.26	103.15921	94.83	104.229	97.53891	95.001	99.366	95.23983
39	1299	1377.87	1.213	521.201	635.662	566.86287	487.863	528.626	498.07961	537.778	496.44	506.76682
40	861.4	279.63	0.951	500.688	499.828	490.25284	407.681	365.272	378.74697	426.821	446.681	428.01598
41	1047.2	524.55	1.266	925.847	848.304	869.33399	636.823	570.129	591.40648	607.365	588.368	585.90917
phenylacetaldehyde dimer	1040.5	511.28998	1.541	90.7	75.056	81.22044	57.807	44.497	50.12896	55.989	52.551	53.1846
n-Nonanal monomer	1104.2	652.86	1.499	1230.216	1157.821	1170.13813	1077.462	1128.154	1080.75184	1023.5	937.926	961.09874
n-Nonanal dimer	1103	649.74	1.937	744.361	620.469	668.7667	502.492	509.195	495.72663	421.927	370.49	388.28433
45	1004.5	445.37997	1.426	121.132	123.673	119.95445	151.45	152.668	149.01782	127.324	114.052	118.27424
46	827	254.08499	1.389	29.236	32.424	30.2134	36.453	44.332	39.58465	31.152	33.081	31.47417
47	902.9	315.705	1.349	27.159	23.026	24.59065	33.506	26.055	29.18489	29.63	20.307	24.46913
48	820.6	249.59999	1.414	128.602	134.531	128.93517	98.681	100.93	97.80939	95.144	92.14	91.76916
49	901.2	313.94998	1.446	38.054	38.384	37.45462	36.361	37.322	36.10467	36.082	35.181	34.91887
50	888	301.08	1.361	36.849	40.259	37.78292	45.22	42.299	42.88431	41.02	36.215	37.84515
ethanol	484.9	102.57	1.047	1253.2	1029.441	1118.49409	953.963	1149.174	1030.53713	1173.78	1267.566	1196.25954
Furfurol monomer	829.7	256.035	1.08	606.093	580.279	581.32228	638.225	678.005	644.9527	633.103	628.976	618.41871
53	908	321.16498	1.575	109.098	97.304	101.13698	113.926	117.079	113.19245	113.605	110.335	109.7306
54	893.9	306.345	1.564	140.827	138.788	137.01135	117.872	109.602	111.46226	90.427	102.506	94.53717
55	814.3	245.31	1.475	159.339	140.551	146.9461	132.231	131.429	129.1934	142.315	125.243	131.10342
56	782.5	224.44499	1.446	395.869	354.065	367.46766	344.232	347.518	338.9575	314.85	332.974	317.43376
57	781.4	223.665	1.415	311.214	308.236	303.5305	313.34	319.763	310.22047	282.378	287.18	279.08342
58	732.4	192.65999	1.312	36.979	43.786	39.57485	68.534	46.987	56.60529	54.435	41.826	47.16789
59	756.4	207.28499	1.449	121.107	108.673	112.5922	98.637	84.334	89.65579	74.812	71.446	71.66642

Compound	RI	Rt [sec]	Dt [RIPrel]	H6-1	H6-2	H6-3	H7-1	H7-2	H7-3	H8-1	H8-2	H8-3
60	783.9	225.42	1.522	168.677	215.119	188.06004	238.36	147.882	189.25858	182.022	123.289	149.60239
1-pentanol dimer	759.5	209.23499	1.52	92.911	83.36	86.37279	88.426	92.692	88.74782	61.096	61.429	60.03725
Acetic acid	574.9	127.725	1.061	1096.573	1357.099	1202.29928	1255.062	998.197	1104.09691	1310.442	1156.797	1208.94711
63	812.6	244.13998	1.282	94.018	94.427	92.33805	82.114	75.259	77.11277	69.695	69.993	68.44712
64	788.5	228.34499	1.557	2176.801	2170.625	2130.23874	2082.713	1933.711	1968.04776	1856.438	1736.032	1760.3103
Z-3-hexen-1-ol dimer	845	267.15	1.507	113.745	105.136	107.25169	79.836	73.904	75.3326	77.187	57.55	66.02113
66	989.4	421.78497	1.247	492.066	454.487	463.81097	486.315	467.689	467.46196	440.546	388.513	406.23891
Ethyl lactate dimer	811.7	243.555	1.539	172.744	162.679	164.35727	146.391	110.405	125.83004	122.024	112.045	114.69381
Benzaldehyde dimer	961.2	383.75998	1.464	1245.34	1179.876	1188.35584	1392.203	1384.756	1360.70991	1147.718	1076.758	1089.99324
Furfurol dimer	829.7	256.035	1.329	1364.889	1251.348	1281.95613	1589.863	1604.95	1565.45837	1398.135	1412.733	1377.32532
70	1002.2	441.47998	1.467	781.882	787.49	768.99228	628.411	776.483	688.39806	791.303	759.754	760.01793
Phenylacetaldehyde monomer	1045.9	522.01495	1.24	1080.688	1121.128	1078.88984	809.006	779.659	778.44585	764.135	819.261	775.86404
72	1092.3	623.61	1.363	1154.532	1193.862	1150.71306	1119.745	1180.377	1127.05978	1205.274	1262.04	1208.98386
73	1103.1	649.935	1.529	939.603	880.138	891.67309	881.962	866.115	856.55773	815.277	861.106	821.42767
74	712.6	181.34999	1.081	95.411	88.464	90.09875	92.626	69.479	79.43145	87.966	79.484	82.0505
75	827.5	254.47499	1.272	57.778	58.923	57.18349	64.915	63.789	63.06496	64.135	69.223	65.34542
Ethyl lactate monomer	814.3	245.31	1.141	87.607	99.439	91.65254	80.594	72.931	75.22725	88.975	71.494	78.62981
77	845	267.15	1.184	717.947	806.341	746.90112	915.189	879.015	879.15996	850.359	879.11	847.43981
Butyl acetate monomer	805.9	239.655	1.239	773.508	783.072	762.7242	753.807	800.911	761.81182	814.227	837.418	809.30605
Ethyl valerate monomer	896.5	309.07498	1.26	433.495	426.881	421.58424	473.967	466.608	460.88175	466.268	467.845	457.71537
Benzaldehyde monomer	960.1	382.395	1.148	790.291	752.056	755.75003	792.283	803.144	781.75923	750.695	708.187	714.85218
81	982.1	411.645	1.45	356.327	327.623	335.1355	256.098	255.435	250.65117	251.47	264.964	253.05266
82	982.4	412.03497	1.476	149.385	138.318	140.97447	83.084	86.453	83.07313	80.252	79.576	78.31572
83	733.1	193.04999	1.335	42.682	35.901	38.50567	36.716	41.154	38.1563	37.614	47.881	41.89255
84	753.6	205.53	1.345	110.043	94.291	100.12366	70.32	81.46	74.3722	100.089	84.207	90.30504
85	876.9	291.91498	1.395	265.147	329.285	291.27168	351.835	347.791	342.81674	364.345	360.488	355.16817
86	958.6	380.44498	1.383	302.12	323.154	306.38426	380.989	378.22	372.01241	370.182	394.746	374.81472
87	961.7	384.34497	1.289	640.481	700.295	656.98024	715.248	718.448	702.51104	726.902	776.09	736.46608
88	1144.4	761.67	1.406	316.718	297.559	300.99573	233.288	240.317	232.06645	225.529	210.212	213.51309

Compound	RI	Rt [sec]	Dt [RIPrel]	H6-1	H6-2	H6-3	H7-1	H7-2	H7-3	H8-1	H8-2	H8-3
89	1144.5	762.06	1.539	265.341	261.785	258.29174	216.235	262.673	234.66492	210.83	237.754	219.80616
90	1104.1	652.47	1.586	275.663	270.803	267.76834	235.283	220.222	223.19745	226.614	229.298	223.39688
E -2-octenal	1062.2	555.75	1.326	381.208	374.068	370.08524	391.752	375.425	375.91673	361.522	356.244	351.70534
92	1059.8	550.68	1.46	290.784	282	280.66416	341.827	319.176	323.89147	264.868	278.974	266.48258
93	1031.8	494.52	1.369	121.64	107.388	112.22372	171.494	177.635	171.07321	142.953	147.653	142.39694
E 2-heptenal	959.5	381.615	1.665	338.621	295.126	310.53603	340.318	369.281	347.70351	298.942	242.474	265.29384
95	961	383.56497	1.563	667.719	594.388	618.43243	856.535	824.479	823.69686	632.601	595.727	601.88072
96	739.7	196.95	0.956	161.138	178.152	166.2521	172.956	150.296	158.39348	167.104	167.421	163.91725
97	800	235.75499	1.586	215.338	209.755	208.29557	206.094	177.435	187.92921	172.519	160.256	163.05975
98	569.2	125.96999	1.174	262.267	276.849	264.16684	306.916	275.958	285.60826	300.772	247.873	268.83605
99	571.7	126.74999	1.214	125.415	123.603	122.01882	113.358	125.107	116.84785	157.645	149.5	150.50105
100	554.3	121.48499	1.196	141.57	134.972	135.50558	122.62	148.316	132.75864	146.502	158.54	149.47058
101	717.2	183.885	1.394	49.258	37.309	42.41783	41.391	57.762	48.58497	39.472	58.444	47.97884
6-methyl-5-hepten-2-one	992	425.49	1.17	186.041	182.419	180.5454	158.606	151.482	151.94312	144.897	147.993	143.5161
103	984.7	415.155	1.15	215.506	201.292	204.23102	264.424	272.519	263.10207	210.402	182.006	192.27992
104	787.3	227.56499	1.376	508.84	631.675	558.85235	607.435	441.996	514.22119	575.781	481.192	517.91677
105	729.8	191.09999	1.51	146.787	130.734	135.98529	117.405	121.608	117.11637	111.842	98.037	102.84071
106	913	326.625	1.412	333.913	377.573	348.62814	430.272	431.592	422.31336	431.322	471.968	442.6121
107	898.4	311.025	1.387	171.764	225.884	194.84752	270.952	245.776	253.19672	239.759	282.838	256.07253
108	891.3	303.81	1.645	187.503	176.871	178.54326	237.561	251.857	239.81482	219.448	211.712	211.2684
Z-3-hexen-1-ol monomer	845.8	267.735	1.227	270.337	272.646	266.06167	214.817	216.797	211.49086	231.794	217.59	220.19816
110	868.1	284.895	1.228	236.203	240.558	233.61289	218.129	198.78	204.28541	203.772	195.319	195.55459
111	845.5	267.53998	1.418	209.117	195.522	198.27311	179.297	184.423	178.2228	155.365	154.524	151.84561
112	965.9	389.805	1.237	135.333	163.402	146.38015	143.647	152.377	145.05176	173.09	194.577	180.15683
113	415.4	86.579994	1.085	183.383	125.177	151.1944	79.69	179.599	127.05161	154.654	164.173	156.22523
114	636.4	148.39499	1.365	293.588	221.586	252.43526	232.466	281.781	251.98103	229.535	222.224	221.36191
Ethyl Acetate	597.4	134.94	1.331	3096.608	2542.643	2763.23299	2451.02	2827.191	2586.32339	2309.203	2343.252	2279.70295
116	582.9	130.26	1.286	1005.873	750.774	860.75703	852.491	1233.182	1021.97977	965.008	1047.699	986.22643
117	569.8	126.16499	1.243	502.121	425.822	454.69207	538.434	645.01	579.88756	543.297	571.065	546.03738

Table 6 GC-IMS data for sample H9

Compound	RI	Rt [sec]	Dt [RIPrel]	H9-1	H9-2	H9-3
1	531.3	114.854996	1.119	1773.123	1775.381	1738.76696
2	532.7	115.244995	1.094	1926.955	1900.862	1875.63033
3	540.3	117.39	1.147	591.619	546.383	557.62098
4	670	161.06999	1.23	236.917	247.41	237.32023
5	728.4	190.31999	1.247	63.944	68.652	64.97204
6	696	172.37999	1.205	1009.359	1023.338	996.02153
7	705.5	177.45	1.156	1273.882	1225.601	1224.74667
8	681.3	165.555	1.317	690.805	629.147	646.77648
1-pentanol monomer	763.2	211.575	1.252	195.116	207.728	197.39356
10	789.5	228.93	1.278	282.362	273.772	272.50566
1-hexanol monomer	871.8	287.81998	1.324	319.062	367.143	336.24045
12	910.5	323.895	1.285	228.692	282.942	250.70066
13	827.8	254.67	1.298	115.699	104.711	108.0009
14	650.2	153.465	1.407	1001.505	1068.076	1014.09469
15	691.9	170.235	1.417	130.667	145.63	135.38553
Butyl acetate dimer	801.8	236.92499	1.615	606.229	706.899	643.43272
17	951.5	371.47498	1.331	52.503	54.793	52.57504
1-hexanol dimer	869.1	285.675	1.654	48.915	66.288	56.44947
19	874.7	290.16	1.703	194.199	280.95	232.82301
Ethyl valerate dimer	893.5	305.955	1.681	1217.477	1593.819	1377.53504
21	908.4	321.555	1.713	183.392	291.386	232.64122
22	1004.3	444.99	1.686	43.548	35.184	38.57868
1-octen-3-one	979.3	407.745	1.275	65.955	67.71	65.49585
24	968.5	393.31497	1.211	28.786	25.303	26.50361
25	941.6	359.38498	1.207	31.622	29.696	30.04582
26	1045.1	520.45496	1.205	229.409	210.148	215.38293
27	1063.6	558.675	1.187	261.852	273.347	262.24751
Methyl benzoate monomer	1095.1	630.435	1.226	1254.907	1165.919	1186.20474
Methyl benzoate dimer	1090.2	618.735	1.6	513.474	426.926	460.796

Compound	RI	Rt [sec]	Dt [RIPrel]	H9-1	H9-2	H9-3
Ethyl hexanoate monomer	1002.3	441.675	1.342	181.546	183.627	178.93477
31	982.4	412.03497	1.386	116.378	117.485	114.59287
32	1027.5	486.525	1.261	49.88	58.948	53.32572
33	915.4	329.15997	1.327	120.885	130.598	123.22667
34	759.5	209.23499	1.298	127.105	132.964	127.43381
Ethyl hexanoate dimer	999.9	437.58	1.818	71.088	85.663	76.80799
36	690.8	169.65	1.18	416.522	436.734	418.09544
37	807.4	240.62999	1.82	38.34	43.533	40.11777
38	1109.8	666.89996	1.26	106.668	89.352	96.0498
39	1299	1377.87	1.213	570.614	518.13	533.48456
40	861.4	279.63	0.951	444.327	415.951	421.53622
41	1047.2	524.55	1.266	609.62	622.721	603.84709
phenylacetaldehyde dimer	1040.5	511.28998	1.541	52.988	53.702	52.2781
n-Nonanal monomer	1104.2	652.86	1.499	1011.491	1023.744	997.26515
n-Nonanal dimer	1103	649.74	1.937	385.852	374.521	372.58277
45	1004.5	445.37997	1.426	131.825	128.019	127.32356
46	827	254.08499	1.389	37.674	35.964	36.08262
47	902.9	315.705	1.349	68.61	61.917	63.95823
48	820.6	249.59999	1.414	94.145	94.069	92.22486
49	901.2	313.94998	1.446	97.764	91.224	92.60412
50	888	301.08	1.361	46.895	45.674	45.35881
ethanol	484.9	102.57	1.047	1487.96	1502.897	1465.51993
Furfurol monomer	829.7	256.035	1.08	715.273	723.086	704.79591
53	908	321.16498	1.575	47.234	60.779	52.92637
54	893.9	306.345	1.564	123.476	139.825	129.01749
55	814.3	245.31	1.475	114.468	118.68	114.24252
56	782.5	224.44499	1.446	265.89	272.976	264.04434
57	781.4	223.665	1.415	265.239	276.903	265.64958
58	732.4	192.65999	1.312	49.023	47.574	47.33253
59	756.4	207.28499	1.449	68.766	72.41	69.17624

Compound	RI	Rt [sec]	Dt [RIPrel]	H9-1	H9-2	H9-3
60	783.9	225.42	1.522	204.264	199.884	198.03252
1-pentanol dimer	759.5	209.23499	1.52	62.139	65.137	62.36524
Acetic acid	574.9	127.725	1.061	1200.199	1152.959	1153.04742
63	812.6	244.13998	1.282	74.228	66.358	68.88714
64	788.5	228.34499	1.557	1889.208	1927.168	1870.02424
Z-3-hexen-1-ol dimer	845	267.15	1.507	53.661	54.803	53.14736
66	989.4	421.78497	1.247	523.681	548.67	525.45199
Ethyl lactate dimer	811.7	243.555	1.539	70.739	88.296	77.92715
Benzaldehyde dimer	961.2	383.75998	1.464	1311.933	1308.031	1283.78236
Furfurol dimer	829.7	256.035	1.329	1919.307	1992.996	1917.02847
70	1002.2	441.47998	1.467	179.865	231.895	201.7624
Phenylacetaldehyde monomer	1045.9	522.01495	1.24	822.826	833.817	811.75507
72	1092.3	623.61	1.363	1226.486	1133.638	1156.46076
73	1103.1	649.935	1.529	795.934	773.92	769.22846
74	712.6	181.34999	1.081	66.025	62.663	63.05712
75	827.5	254.47499	1.272	55.174	50.597	51.82779
Ethyl lactate monomer	814.3	245.31	1.141	86.386	87.776	85.33938
77	845	267.15	1.184	994.53	1034.012	993.98558
Butyl acetate monomer	805.9	239.655	1.239	658.399	686.96	659.22591
Ethyl valerate monomer	896.5	309.07498	1.26	453.669	475.778	455.42903
Benzaldehyde monomer	960.1	382.395	1.148	799.43	803.03	785.2054
81	982.1	411.645	1.45	223.518	212.511	213.65421
82	982.4	412.03497	1.476	63.63	66.46	63.7441
83	733.1	193.04999	1.335	34.74	33.477	33.42633
84	753.6	205.53	1.345	82.085	73.01	75.99655
85	876.9	291.91498	1.395	239.962	264.231	247.05457
86	958.6	380.44498	1.383	398.21	407.015	394.56025
87	961.7	384.34497	1.289	768.106	795.772	766.30022
88	1144.4	761.67	1.406	210.116	210.919	206.30715
89	1144.5	762.06	1.539	221.967	215.518	214.36765

Compound	RI	Rt [sec]	Dt [RIPrel]	H9-1	H9-2	H9-3
90	1104.1	652.47	1.586	210.846	216.838	209.56516
E -2-octenal	1062.2	555.75	1.326	349.044	364.793	349.78013
92	1059.8	550.68	1.46	285.318	287.999	280.92533
93	1031.8	494.52	1.369	157.35	172.681	161.71519
E 2-heptenal	959.5	381.615	1.665	246.801	265.49	251.02259
95	961	383.56497	1.563	756.509	779.586	752.68655
96	739.7	196.95	0.956	138.287	146.14	139.36923
97	800	235.75499	1.586	149.712	165.099	154.25739
98	569.2	125.96999	1.174	291.865	297.873	288.97162
99	571.7	126.74999	1.214	147.228	172.684	156.75688
100	554.3	121.48499	1.196	118.592	126.636	120.16172
101	717.2	183.885	1.394	32.925	41.02	36.23305
6-methyl-5-hepten-2-one	992	425.49	1.17	115.902	100.311	105.94437
103	984.7	415.155	1.15	224.08	214.786	215.04434
104	787.3	227.56499	1.376	613.046	607.559	598.09645
105	729.8	191.09999	1.51	109.811	96.613	101.14776
106	913	326.625	1.412	284.421	340.34	306.13289
107	898.4	311.025	1.387	503.45	499.444	491.41806
108	891.3	303.81	1.645	185.277	208.451	192.92672
Z-3-hexen-1-ol monomer	845.8	267.735	1.227	181.166	193.616	183.64318
110	868.1	284.895	1.228	156.554	146.927	148.70569
111	845.5	267.53998	1.418	177.305	177.356	173.78389
112	965.9	389.805	1.237	174.155	183.237	175.12208
113	415.4	86.579994	1.085	132.977	169.309	148.12014
114	636.4	148.39499	1.365	237.18	248.114	237.79406
Ethyl Acetate	597.4	134.94	1.331	3001.032	3160.273	3019.03945
116	582.9	130.26	1.286	925.18	1002.2	944.4162
117	569.8	126.16499	1.243	467.562	499.168	473.6977