

**Supplemental data I.** Results of putative identification of 70 volatiles represented in Table 2 of the text. For each compound 5 first matching hits derived from the NIST library are given with corresponding match value and probability. The identity of compounds depicted in bold were confirmed by authentic chemical standards.

GC/MS data			NIST library matching result		
compound#	R.T., min	selective ion, m/z	Library hit	match value, maximal match value = 1000	probability, %

### Phenylpropanoid volatiles

1	21.55	122	<b>Salicylaldehyde</b>	<b>838</b>	<b>26</b>
			Salicylaldehyde	825	26
			Propanoic acid, 3-chloro-,4-formy	815	18.4
			4-hydroxybenzaldehyde	813	16.9
			3-hydroxybenzaldehyde	810	16.9
2	23.06	81	<b>Guaiacol</b>	<b>924</b>	<b>73.7</b>
			Guaiacol	919	73.7
			Guaiacol	914	73.7
			p-Guaiacol	892	19.8
			Guaiacol	888	73.7
3	26.89	120	<b>Methyl salicylate</b>	<b>960</b>	<b>91.2</b>
			Methyl salicylate	948	91.2
			Methyl salicylate	943	91.2
			Methyl salicylate	930	91.2
			Methyl salicylate	925	91.2
4	29.32	120	<b>Ethyl salicylate</b>	<b>951</b>	<b>96.2</b>
			Ethyl salicylate	948	96.2
			Ethyl salicylate	919	96.2
			2-ethoxy-benzoic acid	801	2.7
			Ethyl salicylate	769	96.2
5	31.9	164	<b>Eugenol</b>	<b>920</b>	<b>52.2</b>
			Eugenol	887	52.2
			Isoeugenol	886	13.4
			Eugenol	882	52.2
			3-Allyl-6-methoxyphenol	881	10.8

### Phenolic volatiles

6	10.79	91	<b>Toluene</b>	<b>953</b>	<b>31.9</b>
			1,3,5-Cycloheptatriene	943	22.5
			Toluene	942	31.9
			Toluene	936	31.9
			Cyclobutene, 2-propenylidene	936	32
7	14.45	91	<b>Ethylbenzen</b>	<b>946</b>	<b>69.5</b>
			Ethylbenzen	939	69.5
			Ethylbenzen	922	69.5
			Ethylbenzen	917	69.5
			o-Xylene	885	11.2

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8	15.61	104	<b>Styrene</b> Styrene Benzocyclobutane Benzocyclobutane Styrene	<b>964</b> 963 954 943 939	<b>44.3</b> 44.3 31.3 31.3 44.3
9	18.05	91	<b>1-Phenylpropane</b> 1-Phenylpropane N-Benzyl-2-phenylethylamine Benzylethanolamine Benzylethanolamine	<b>934</b> 924 900 888 881	<b>49.6</b> 49.6 13.5 9.01 9.01
10	18.34	106	<b>Benzaldehyde</b> Benzaldehyde Benzaldehyde Benzaldehyde Phenylglyoxal	<b>944</b> 924 919 904 827	<b>72</b> 72 72 72 4.1
11	18.55	94	<b>Phenol</b> Phosphoric acid, (p-hydroxyphen Phenol Phenol Phenol	<b>931</b> 914 911 910 910	<b>55</b> 30 55 55 55
12	19.11	118	<b>o-Methylstyrene</b> 2-Phenyl-3-buten-1-ol 3,5-Diphenyl-1-pentane o-Methylstyrene $\beta$ -Methylstyrene	<b>705</b> 680 671 665 661	<b>14.3</b> 13.2 9.57 14.3 6.76
13	19.24	103	<b>Benzonitrile</b> Benzonitrile Benzonitrile Tricyclo [3.1.0.0[2,4]]hex-3-ene-3 Benzonitrile	<b>841</b> 834 825 819 812	<b>58.3</b> 58.3 58.3 23 58.3
14	20.8	117	<b>2-Phenyl-3-buten-1-ol</b> Z- $\beta$ -Methylstyrene 3,5-Diphenyl-1-pentane Benzen, cyclopropyl Benzocyclopentane	<b>782</b> 774 768 768 767	<b>16.4</b> 12.3 5.6 4.7 1.9
15	20.94	108	<b>Benzyl alcohol</b> Benzyl alcohol Benzyl alcohol N-Benzylloxycabonyl-L-tyrosine 1-Phenyl-1,2-propanediol	<b>942</b> 932 931 914 874	<b>81.6</b> 81.6 81.6 4.3 1.3
16	21.43	120	<b>Phenylacetaldehyde</b> Phenylacetaldehyde Phenylacetaldehyde Phenylacetaldehyde Phtalan	<b>950</b> 944 920 913 876	<b>70.6</b> 70.6 70.6 70.6 9.4
17	22.09	107	<b>p-Cresol</b> p-Cresol m-Cresol p-Cresol p-Cresol	<b>951</b> 940 936 934 933	<b>50.3</b> 50.3 30.5 50.3 50.3
18	23.63	105	<b><math>\alpha</math>-Phenylpropionaldehyde</b> $\alpha$ -Phenylpropionaldehyde $\alpha$ -Methyl styrene oxide 1-Nitro-1-phenylethane Toluene, p-propyl-	<b>862</b> 854 821 796 793	<b>54.4</b> 54.4 12.4 3.78 3.34

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19	23.95	91	<b>Phenylethanol</b> Phenylethanol Phenylethanol Benzyl hyrazide Benzyl hyrazide	<b>944</b> 928 926 824 820	<b>87.6</b> 87.6 87.6 4.59 4.59
20	24.82	117	<b>Phenylacetonitrile</b> o-Tolunitrile p-Tolylisonitrile m-Tolunitrile Phenylacetonitrile	<b>856</b> 827 816 814 812	<b>43.8</b> 12.4 8.52 7.85 43.8
21	25.66	92	<b><math>\beta</math>-Phenylpropionaldehyde</b> $\beta$ -Phenylpropionaldehyde n-Butylbenzene n-Butylbenzene n-Butylbenzene	<b>876</b> 832 816 806 806	<b>46.2</b> 46.2 26.6 26.6 26.6

### Leucine and Isoleucine derived volatiles

22	6.96	44	<b>Butanal, 3-methyl-</b> Butanal, 3-methyl- Butanal, 3-methyl- Butanal, 3-methyl- Pentanal	<b>837</b> 825 793 781 774	<b>82.5</b> 82.5 82.5 82.5 16.7
23	7.21	57	<b>Butanal, 2-methyl-</b> Butanal, 2-methyl- Butanal, 2-methyl- 1-Propene, 3-ethoxy- Formic acid, 2-propenyl ester	<b>887</b> 873 853 831 832	<b>74.1</b> 74.1 74.1 4.73 3.81
24	9.32	43	<b>1-Butanol, 3-methyl-</b> 1-Butanol, 3-methyl- 1-Butanol, 3-methyl- 2(3H)-Furanone, dihydro-3,5-dim 1-Pentanol	<b>894</b> 891 873 815 815	<b>54.7</b> 54.7 54.7 6.23 6.23
25	9.5	57	<b>1-Butanol, 2-methyl-</b> 1-Butanol, 2-methyl-, (S)- 1-Butanol, 2-methyl-, ( $\pm$ )- 1-Butanol, 2-methyl- 1-Butanol, 2-methyl-	<b>922</b> 897 887 872 870	<b>62.2</b> 19 13.4 62.2 62.2
26	9.77	42	2-Butenal, 2-methyl-, (E)- 2-Butenal, 2-methyl- 2-Butenal, 2-methyl- 2-Butenal, 2-methyl- 2-Butenal, 2-methyl-	922 913 903 902 892	48.4 29.4 29.4 29.4 29.4
27	12.77	60	<b>Butanoic acid, 3-methyl-</b> Butanoic acid, 3-methyl- Pentanoic acid, 3-methyl- Pentanoic acid, 3-methyl- Hexanoic acid	<b>922</b> 908 807 793 768	<b>91.6</b> 91.6 5.42 5.42 1.23
28	15.85	41	3-Methylbutanol nitrite Pentane, 1-nitro- 1-Butanol, 2-ethyl- Pentane, 1-nitro- 1-Pentanol, 2-methyl-	835 800 796 795 788	22 13.3 12.3 13.3 9.18

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29	16.39	41	Cyclopentane, nitro-	778	30
			1-Pentene, 5-nitro-	753	9.14
			Cyclopentanemethanol	752	8.78
			1-Butene, 2-methyl-4-[(3-methyl-2-butyl)oxy]-	733	4.26
			2-Buten-1-ol, 3-methyl-, acetate	732	4.1
30	17.42	43	Amyl nitrite	917	65.3
			Pentane, 1-nitro-	897	29.8
			Pentane, 1-nitro-	884	29.8
			1,6-Heptadien-4-ol	759	1.05
			Hexane, 1-nitro-	748	0.72
31	21.04	99	<b>2-Isobutylthiazole</b>	<b>902</b>	<b>97.3</b>
			2-Isobutylthiazole	894	97.3
			2-Isobutylthiazole	839	97.3
			2-Isobutylthiazole	811	97.3
			2-Propylthiazole	725	1.86

### Lipid derived volatiles

32	13.95	82	<b>Z-3-Hexenol</b>	<b>899</b>	<b>32</b>
			3-Hexen-1-ol	897	29.5
			3-Hexen-1-ol, (E)-	888	21.4
			3-Hexen-1-ol, (Z)-	883	32
			3-Hexen-1-ol, (Z)-	883	32
33	7.67	57	<b>1-Penten-3-ol</b>	<b>903</b>	<b>71.7</b>
			1-Penten-3-ol	898	71.7
			1-Penten-3-ol	893	71.7
			1-Penten-3-ol	854	71.7
			1-Ethylcyclopropanol	821	7.31
34	7.83	55	<b>1-Penten-3-one</b>	<b>882</b>	<b>85.2</b>
			1-Penten-3-one	878	85.2
			1H-Imidazole, 4,5-dihydro-2-methyl-	765	4.34
			2(5H)-Furanone	751	2.89
			2(5H)-Furanone	744	2.89
35	8.18	44	<b>Pentanal</b>	<b>883</b>	<b>89.6</b>
			Pentanal	874	89.6
			Pentanal	862	89.6
			Butanal, 3-methyl-	777	6.02
			Butanal, 3-methyl-	774	6.02
36	8.37	81	<b>Furan, 2-ethyl-</b>	<b>934</b>	<b>85.8</b>
			Furan, 2-ethyl-	907	85.8
			2,4-Hexadienal, (E,E)-	789	2.57
			Cyclopentene, 1,5-dimethyl	786	2.27
			Cyclopentene, 4,4-dimethyl-	770	1.31
37	10.2	55	<b>2-Pentenal, (E)-</b>	<b>926</b>	<b>50.4</b>
			2-Pentenal, (E)-	902	50.4
			2-Pentenal, (E)-	882	50.4
			Cyclobut-1-enylmethanol	879	10.5
			4-Pentenal	871	7.86
38	10.51	42	<b>1-Pentanol</b>	<b>895</b>	<b>72.4</b>
			1-Pentanol	887	72.4
			1-Pentanol	887	72.4
			1-Pentanol	872	72.4
			1-Pentanol	854	72.4

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39	10.65	57	<b>2-Penten-1-ol, (Z)-</b> 2-Penten-1-ol, (Z)- 2-Penten-1-ol, (E)- Cyclopentanol 2-Penten-1-ol, (Z)-	<b>891</b> 869 856 854 852	<b>59.1</b> 59.1 14.8 13.7 59.1
40	11.76	80	<b>3-Hexenal, (Z)-</b> 4-Pentenal, 2-methyl- 2-Hexenal 1-Pentene, 2,3-dimethyl- 2-Hexenal	<b>847</b> 802 787 781 774	<b>46.8</b> 9.97 6.04 4.75 6.04
41	11.83	72	<b>Hexanal</b> Hexanal Hexanal Hexanal Cyclobutanol, 2-ethyl-	<b>856</b> 843 836 805 716	<b>91.5</b> 91.5 91.5 91.5 3.11
42	13.6	41	<b>2-Hexenal</b> 2-Hexenal 2-Hexenal, (E)- 2-Hexenal, (E)- 2-Hexenal, (E)-	<b>904</b> 897 891 896 890	<b>35.6</b> 35.6 23 23 23
43	13.9	98	<b>2-Hexenal, (E)-</b> 2-Hexenal, (E)- 2-Hexenal, (E)- 2-Hexenal 2-Hexenal	<b>944</b> 943 940 938 899	<b>45.5</b> 45.5 45.5 38.5 38.5
44	14.36	56	<b>1-Hexanol</b> 1-Hexanol 1-Hexanol 1-Hexanol Formic acid	<b>932</b> 930 928 926 873	<b>53.2</b> 53.2 53.2 53.2 9.62
45	15.75	70	Heptanal Heptanal Heptanal Heptanal Hexanal, 3-methyl-	898 882 871 870 740	92.7 92.7 92.7 92.7 2.35
46	16.13	81	<b>2,4-Hexadienal, (E,E)-</b> 2,4-Hexadienal, (E,E)- 2,4-Hexadienal, (E,E)- Furan, 2-ethyl- Furan, 2-ethyl-	<b>938</b> 915 913 878 860	<b>54.2</b> 54.2 54.2 9.62 9.62
47	17.91	41	<b>2-Heptenal, (E)-</b> 2-Heptenal, (Z)- 2-Heptenal, (E)- 4-Pentenal, 2-ethyl- 1-Hexene, 3,5-dimethyl-	<b>952</b> 895 895 859 845	<b>66.7</b> 12.5 12.5 3.09 1.93
48	19.26	81	<b>Furan, 2-pentyl-</b> Furan, 2-pentyl- Furan, 2-pentyl- 2,4-Nonadienal, (E,E)- 2,4-Nonadienal, (E,E)-	<b>925</b> 893 866 780 764	<b>91.3</b> 91.3 91.3 2.73 2.73
49	19.44	81	<b>2,4-Heptadienal, (E,E)-</b> 1-Hexyne, 5-methyl- 1-Hexyne, 5-methyl- 1-Hexyne, 5-methyl- 4-Ethylcyclohexanol	<b>721</b> 713 709 701 688	<b>31.6</b> 23.6 23.6 23.6 7.2

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50	20.5	57	<b>1-Hexanol, 2-ethyl-</b>	<b>939</b>	<b>65.2</b>
			1-Hexanol, 2-ethyl-	944	65.2
			1-Hexanol, 2-ethyl-	926	65.2
			1-Hexanol, 2-ethyl-	918	65.2
			2-Propyl-1-pentanol	894	14.9

### Open chain carotenoid derivatives volatiles

51	18.99	43	<b>5-Hepten-2-one, 6-methyl-</b>	<b>919</b>	<b>76.2</b>
			5-Hepten-2-one, 6-methyl-	918	76.2
			5-Hepten-2-one, 6-methyl-	891	76.2
			1-Hepten-6-one, 2-methyl-	882	18.6
			3-Hepten-2-one, 5-methyl-	781	1.35
52	19.17	95	<b>5-Hepten-2-ol, 6-methyl-</b>	<b>810</b>	<b>43.5</b>
			dl-6-Methyl-5-hepten-2-ol	803	33.3
			5-Hepten-2-ol, 6-methyl-	793	43.5
			5-Hepten-2-ol, 6-methyl-	782	43.5
			6-Hepten-1-ol, 2-methyl-	778	10.2
53	20.07	43	<b>5-Hexen-2-one, 5-methyl-3-methyl-</b>	<b>757</b>	<b>27.8</b>
			Ethanone, 1-(1-cyclohexen-1-yl)-	756	26.8
			Ethanone, 1-(2-methyl-1-cyclohexen-1-yl)-	749	20.5
			Ethanone, 1-(1-cyclohexen-1-yl)-	727	26.8
			Ethanone, 1-(1-cyclohexen-1-yl)-	727	26.8
54	22.32	105	<b>Acetophenone</b>	<b>928</b>	<b>53.8</b>
			Acetophenone	925	53.8
			Acetophenone	916	53.8
			Acetophenone	904	53.8
			Acetophenone	901	53.8
55	23.41	109	<b>6-Methyl-3,5-heptadiene-2-one</b>	<b>916</b>	<b>43.8</b>
			Ethanone, 1-(2-methyl-1-cyclohexen-1-yl)-	910	34.4
			Ethanone, 1-(2-methyl-1-cyclohexen-1-yl)-	903	34.4
			6-Methyl-3,5-heptadiene-2-one	893	43.8
			Ethanone, 1-(2-methyl-1-cyclohexen-1-yl)-	879	34.4
56	26.51	119	<b>Acetophenone, 4'-methyl-</b>	<b>913</b>	<b>34.6</b>
			Acetophenone, 4'-methyl-	908	34.6
			Acetophenone, 3'-methyl-	905	25.8
			Acetophenone, 3'-methyl-	896	25.8
			Acetophenone, 3'-methyl-	887	25.8
57	28.1	69	<b><math>\beta</math>-Citral</b>	<b>906</b>	<b>52.1</b>
			$\beta$ -Citral	887	52.1
			$\alpha$ -Citral	856	20.6
			Citral	791	19
			$\alpha$ -Citral	785	20.6
58	28.98	41	<b><math>\alpha</math>-Citral</b>	<b>941</b>	<b>67.4</b>
			$\alpha$ -Citral	927	67.4
			Citral	914	19.8
			Citral	913	19.8
			Citral	906	19.8
59	34.36	43	<b>Geranyl acetone</b>	<b>907</b>	<b>39</b>
			trans-Geranylacetone	904	34.5
			cis-Geranylacetone	893	23.6
			trans-Geranylacetone	890	39
			trans-Geranylacetone	881	39

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60	38.06	69	Pseudoionone	711	55.9
			Pseudoionone	668	27.2
			1,4-Hexadiene, 3,3,5-trimethyl-	616	5.42
			1,5-Heptadiene, 2,6-dimethyl-	585	1.47
			1,5-Heptadiene, 2,6-dimethyl-	582	1.47

## Terpenoids

61	20.9	68	<b>(-)-Limonene</b>	<b>626</b>	<b>20.1</b>
			D-Limonene	617	14.6
			(±)-Limonene	610	11.2
			D-Limonene	609	14.6
			Limonene	608	10.3
62	22.44	59	<b>cis-Linalool Oxide</b>	<b>876</b>	<b>36.7</b>
			α-Methyl-α-[4-methyl-3-pentenyl]	866	25.9
			2-Furanmethanol, 5-ethenyltetra	849	14.1
			cis-Linalool Oxide	847	36.7
			Linalool oxide	835	8.85
63	22.99	59	<b>E-Linaloloxide</b>	<b>799</b>	<b>26.6</b>
			Z-Linalool Oxide	793	20.9
			E-Linaloloxide	792	20.1
			Z-Linaloloxide	773	9.75
			Linalool oxide	770	8.61
64	24.91	93	Ocimenol	<b>821</b>	<b>56.1</b>
			4-Thujanol	730	4.74
			τ-Terpinen	726	4
			Cyclopropane, 1,1-dimethyl-2-(3-	722	3.38
			α-Fenchene	720	3.12
65	26.39	43	p-Cymen-8-ol	<b>863</b>	<b>87.8</b>
			p-Cymen-8-ol	855	87.8
			p-Cymen-8-ol	815	87.8
			1-(2,4-Dimethylphenyl)ethanol	764	6.65
			α,2,5-Trimethylbenzyl alcohol	741	2.43
66	26.69	93	<b>α-Terpineol</b>	<b>889</b>	<b>41.7</b>
			α-Terpineol	883	24
			α-Terpieol	881	22.2
			α-Terpineol	869	41.7
			α-Terpieol	864	22.2
67	29.92	79	2-Caren-10-al	718	23.2
			Benzenemethanol, à-propyl-	702	13.4
			3-Nonen-5-yne, 4-ethyl-	696	10.5
			1,3-Cyclohexadiene-1-carboxalde	694	9.68
			3-Nonen-5-yne, 4-ethyl-, (E)-	690	8.18

## Cyclic carotenoid derivatives

68	22.06	82	α-Isophoron	801	55.1
			α-Isophoron	800	55.1
			1H-Pyrazole, 4,5-dihydro-5,5-dim	791	38.9
			α-Isophoron	790	55.1
			α-Isophoron	757	55.1

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69	27.8	152	<b><math>\beta</math>-Cyclocitral</b>	<b>878</b>	<b>59.4</b>
			$\beta$ -Cyclocitral	870	59.4
			3-Isopropylidene-5-methyl-hex-4-	825	11.7
			3-Cyclohexene-1-carboxaldehyde	806	5.7
			3-Cyclohexene-1-carboxaldehyde	802	5.7
70	32.82	121	<b><math>\beta</math>-Damascenone</b>	<b>910</b>	<b>52.8</b>
			$\beta$ -Damascenone	909	52.8
			E- $\beta$ -Damascenone	906	44.6
			$\beta$ -Damascenone	893	52.8
			$\beta$ -Damascenone	891	52.8
72	35.74	177	<b><math>\beta</math>-Ionone</b>	<b>851</b>	<b>43.8</b>
			E- $\beta$ -Ionone	848	38.7
			$\beta$ -Ionone	841	43.8
			E- $\beta$ -Ionone	837	38.7
			E- $\beta$ -Ionone	815	38.7