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Discrimination of Green, Oolong, and Black Teas by GC-MS Analysis of Characteristic Volatile Flavor Compounds

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Abstract

Tea is one of the most consumed beverages in the world and its quality is influenced by geographical origin and production methods. This study focuses on the volatile aroma components of 38 tea products from China, Japan, Indonesia, Sri-Lanka, and Chinese Taipei; among them 7 green teas, 13 oolong teas, and 18 black teas. The volatiles were extracted from the infusions using PorapakQ-resin, concentrated, and analyzed by gas chromatography-mass spectrometry. The components were identified by authentic reference compounds or preliminary based on their mass spectra. Different manufacturing processes yield different blends of aroma compounds. In general, the contents of total volatiles, aliphatics, aromatics, and terpenoids increased with the fermentation degree, whereas jasmine lactone and indole were the highest in oolong teas. Some particular manufacturing processes, for example, the use of tea leaves infested by the tea green leafhopper, lead to higher contents of volatiles in final products as in Oriental Beauty oolong tea. The relative peak areas determined for 82 volatiles were the basis for the statistical analysis and highlight the potential of multivariate analysis to distinguish tea samples of different categories.

Keywords

Aroma, *Camellia sinensis*, Fermentation, Clustering Analysis, Tea

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1. Introduction

Tea (*Camellia sinensis*) is a plant commercially grown for beverage production. Until now, more than 300 different kinds of tea are produced from the leaves of *C. sinensis* by different fermentation processes. Commonly teas are classified based on the manufacturing process and can be divided up into six major families, including non-fermented green tea, slightly fermented white tea, semi-fermented oolong tea, fully fermented black tea, post fermented yellow tea, and dark (red) tea (**Figure 1**). White tea, yellow tea, and dark tea are characteristic Chinese teas and particularly popular in China, whereas green tea, oolong tea, and black tea are well-known all around the world and in particular focus of this study. From a viewpoint of tea quality evaluation, tea aroma is one of the main sensory properties which are decisive in selection, acceptance and ingestion of final tea products. Formation of tea aroma is influenced by different manufacturing processes. For example, the particular manufacturing process of oolong tea gives a unique floral, fruity, and jasmine-like aroma [1] [2]. The aroma compounds of tea such as green tea, oolong tea and black tea have been individually investigated by gas chromatography-mass spectrometry (GC-MS) or GC-olfactometry (GC-O) [3]-[7]. In addition various approaches were employed for the discrimination of teas from different geographical origins such as high performance liquid chromatography [8], capillary electrophoresis [9] or electronic nose [10].

In our study, we collected more than 38 kinds of tea products including green teas, oolong teas, and black teas from different production areas, investigated their volatile compounds to study the different manufacturing processes on the tea aroma profiles as well as relationships between particular processes and tea aroma compounds**.** We aimed to develop a fast method to determine the origin based on profiling of volatiles by GC-MS and statistical analysis.

2. Experimental

2.1. Tea Samples

In total 38 tea products of high grade were obtained from tea exporters or research centers from China, Japan, Indonesia, Sri-Lanka, and Chinese Taipei; among them 7 green teas, 13 oolong teas, and 18 black teas. Supplementary **Table S1** summarizes names, origin, and other characteristics of tea samples investigated in this study.

2.2. Analysis of Tea Volatile Compounds by GC-MS

Deionized hot water (40 mL, 80˚C) was added to 2 g of the tea product. After 5 min the leaves were removed by nylon filter and small residues by centrifugation at 3000 g for 10 min. 25 mL of the supernatant were passed through a 2 mL PorapakQ-cartridge, conditioned with diethyl ether (5 × 4 mL), methanol (4 mL), and water (4 mL). The cartridge was washed with 3 mL of deionized water prior elution of the volatile compounds with 3 mL

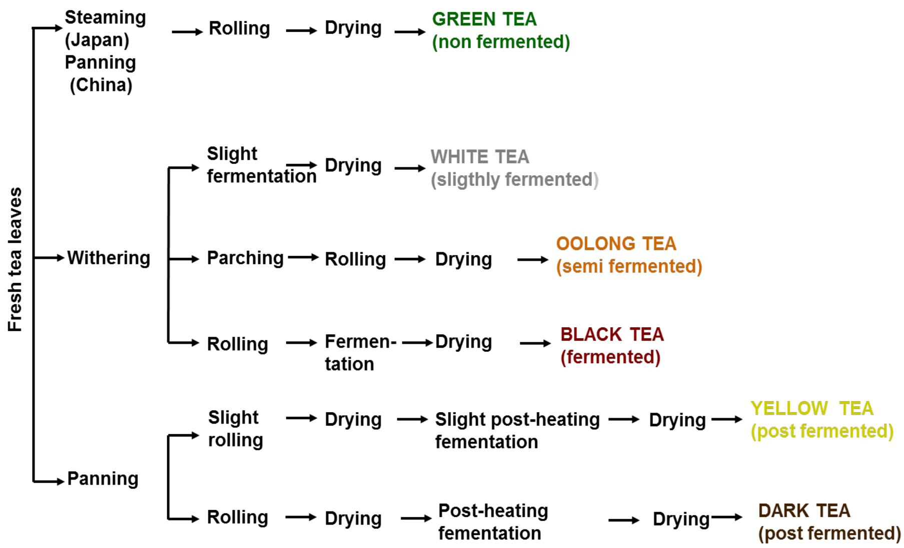


Figure 1. Simplified production processes of various kinds of tea products.

iso-pentane: diethyl ether (1:1, v/v). For relative quantification ethyl decanoate (54.1 pmol) was added as an internal standard and the organic layer dried over anhydrous sodium sulfate. The eluate was concentrated to 100 µL in a stream of nitrogen. One µL concentrate was subjected to GC-MS analysis for identification and relative quantification of the volatiles. Splitless injection mode was used with a splitless time of 1 min and an injector temperature of 230˚C. Helium was the carrier gas with a velocity of 1.7 $mL \cdot min^{-1}$. The GC was equipped with a capillary SUPELCOWAX™ 10 column (30 m × 0.25 mm i.d. and 0.25 µm film thickness). The GC oven was maintained at 50˚C for 3 min and then heated at a rate of 3˚$C \cdot min^{-1}$ to 150˚C followed by a heating rate of 20˚C min^{-1} to 240˚C and kept at this temperature for 20 min. The mass scan range was m/z 50 - 300 and the electric potential was set to EI 70 eV.

2.3. Statistical Analysis

Peak areas of volatiles detected between 4.5 and 58 min were extracted from the mass chromatograms and relative concentrations calculated using the internal standard ethyl decanoate. Clustering analysis by STATISTICA (StatSoft, Inc. (2013). data analysis software system, version 12. www.statsoft.com) was employed for the visualization of the datasets. In this work, 82 volatiles in 38 teas were taken into account. Components identified solely in one tea were excluded from the statistical analysis.

3. Results and Discussion

Compositions of tea products have been investigated by many researchers. Phenolic constituents, organic acids, caffeine, and volatiles are key chemical components defining taste and flavor.

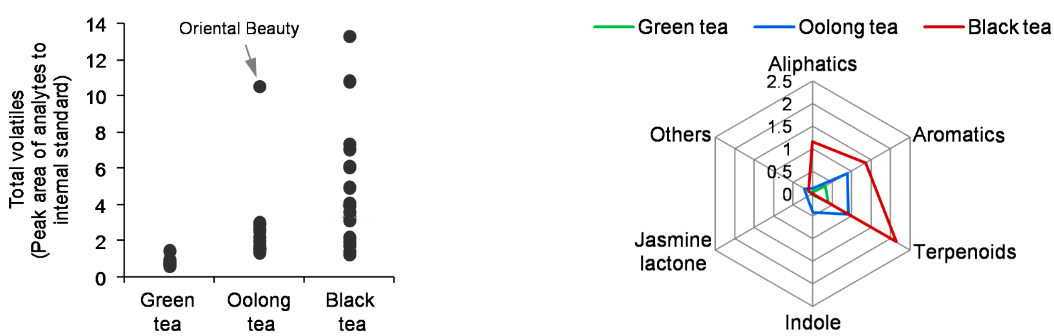
Flavor as a key parameter for tea quality is greatly influenced by brewing temperature, brewing time, extraction methods, and many other factors.

In this study we compared the volatile profiles of green teas, oolong teas, and black teas using equal extraction conditions for all samples. Therefore, our results represent differences mainly caused by manufacturing processes (**Figure 1**) and variation of raw materials including the geographic origin.

Based on the observations on volatile compounds of 38 tea samples (**Table S1**) including green teas (non-fermented), oolong teas (semi-fermented), and black teas (fully fermented), the contents of total volatiles, aliphatics, aromatics, and terpenoids increased with the fermentation degree (**Figure 2(a)** & **Figure 2(b)**).

Clustering analysis was performed to discriminate between tea samples of different categories. As a result of the statistical analysis we could obtain clusters of the different tea categories and distinguish samples according to the origin (**Figure 3**).

In general, the aroma profiles of black teas and oolong teas are more complex than the ones of green teas. In green tea fewer volatiles can be found and among the 200 volatiles about 30 compounds essentially contribute to the typical green tea aroma [5] [6]. Besides short chained alcohols and aldehydes, geraniol, linalool, 2-phenylethanol, benzyl alcohol, indole, and coumarin lead to green tea aroma. In black tea infusions about 600 constituents have been identified and 41 compounds importantly contribute to the aroma of black tea infusions [11].



(a) (b)

Figure 2. Comparisons of total volatile contents (a) and classified volatiles of green teas, oolong teas, and black teas (**Tables S1-S4**). Total volatiles contents were represented as area ratio of volatiles to internal standard (ethyl decanoate); (b) The average values of classified volatiles of green teas, oolong teas and black teas.

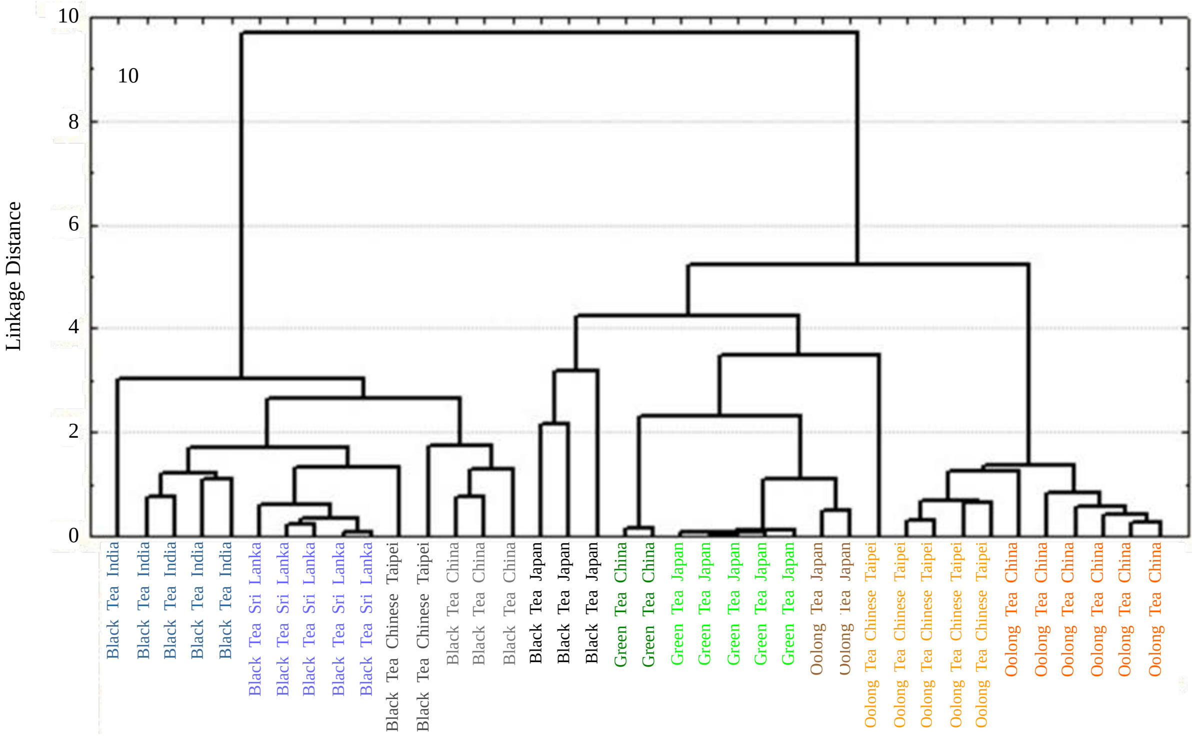


Figure 3. Clustering analyses of the relative peak areas (TIC, mass range *m*/*z* 50 - 300, 82 compounds) of 38 teas (**Table S1**).

Several of these important aroma compounds have been found in all kinds of black tea, among them *Z*-3-hexen-1-ol, linalool and its oxides, geraniol, and 2-phenylethanol contributing to the green, citrus-like, rose-like and honey-like notes, respectively. Linalool and its oxides, benzylalcohol, and 2-phenylethanol were detected as volatiles in all oolong teas. Although contents of most volatiles in black teas are higher than oolong teas and green teas, jasmine lactone and indole were the highest in oolong teas. Both volatiles possess jasmine-like floral and fruity fragrances and importantly contribute to oolong tea aroma [12]. This result is identical with previous reports [13]. Methyl salicylate, previously described as characteristic aroma component of oolong tea, has been only found in some teas of Chinese Taipei (**Table S1** No. 7, 8, and 10) or Japanese (**Table S1** 12 and 13) origin [14].

Many aroma compounds occur as glycosidic precursors in fresh tea leaves [15], and they are hydrolyzed by endogenous glycosidases during the manufacturing processes of withering, rolling, and fermentation [1] [2] [16]. During the production of green teas, plucked fresh tea leaves are steamed or pan-fired to inactivate activity of enzymes including glycosidases related to hydrolysis of glycosidically bound volatiles. In contrast, endogenous enzymatic reactions occur in the several processes of oolong teas and black teas, which results in the accumulation of aroma compounds such as aliphatics, aromatics, and terpenoids in final products (**Figure 2(b)**). During the rolling process of black tea, the structure of the leaf cells is disrupted and the contents of the cells are completely mixed, so the hydrolysis of glycosidically bound aroma precursors plays a major role in the formation of black tea aroma [1]. In contrast, in the processes of oolong teas, one or more biosynthetic pathways, such as the formation of jasmine lactone and indole, might take priority over the hydrolysis of glycosidically bound aroma precursors, although the mechanism for the formation of the two volatiles has not yet been clarified [2]. In the sensory evaluation, oolong teas are generally considered to possess more pleasant flavor than black teas, although these contain higher contents of tea volatiles. This suggests that some characteristic aroma compounds are produced during the manufacturing process of oolong tea. Alive time of tea leaves in the process of oolong tea is much longer time than that in the process of black tea [17]. Therefore, tea leaves during oolong tea manufacturing process are exposed longer to various stresses including plucking (wounding), solar withering (drought, heat, and UV radiation), indoor withering (drought), and turn over (wounding) [18]. In addition, biotic stress such as insect infestation is involved in the oolong tea manufacturing. A typical example is a famous Formosa oolong tea (Oriental Beauty) that has a unique aroma like ripe fruits and honey. It contains the highest content of total volatiles among the oolong teas (**Figure 2(a)**). This may be due to the formation of unique volatiles in tea leaves under insect attack [18]. In the Oriental Beauty manufacturing process, one of the most characteristic factors is the use of tea leaves infested by the tea green leafhopper. It has been reported that formations of many volatiles in tea leaves can be induced by insect attack [19] [20]. Taken together, the aroma formation in tea leaves during the manufacturing process may be the result of defense responses of tea leaves against various stresses. Hence, more detailed molecular studies on stress-induced volatile formation during the tea manufacturing process will provide an important basis for improvement of flavor quality of other teas.

4. Conclusion

In this study, a comprehensive comparison of aroma profiles of green teas, oolong teas, and black teas collected from different production areas was performed. Fermentation intensity influences the quantity of most tea volatiles during the manufacturing process. Besides fermentation, some particular stress-related manufacturing processes, for example during the production of oolong tea, result in the formation of some characteristic tea volatiles such as jasmine lactone or indole. These results will contribute to our further understanding of the effects of different manufacturing processes on tea aroma profile, and provide essential information for further development of aroma-enriched tea products. Moreover, this study could form the basis for authenticity studies of tea products.

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Supplement

Table S1. Classification and geographical origin of tea samples.

No.	Commercial name	Tea type	Origin	Others characteristics
1	Dahongpao	Oolong	China	Roasted
2	Buzhichun	Oolong	China	Roasted
3	Rougui	Oolong	China	Roasted
4	Yunxiang 999	Oolong	China	Pellet type
5	Tieguanyin AAA	Oolong	China	Pellet type
6	Nashiyama	Oolong	Chinese Taipei	Roast, high mountain, pellet type
7	Nashiyama	Oolong	Chinese Taipei	High mountain, pellet type
8	Kouzancha	Oolong	Chinese Taipei	High mountain, organic, pellet type
9	Bunzanhoushycha	Oolong	Chinese Taipei	
10	Oriental Beauty	Oolong	Chinese Taipei	
11	Shikicha	Oolong	Chinese Taipei	Pellet type
12	Shizu 7132	Oolong	Japan	
13	Benifuuki	Oolong	Japan	
14	Zhuangyuanhong	Green	China	
15	Baichazu	Green	China	
16	Yabukita	Green	Japan	
17	Kousyun	Green	Japan	
18	Tsuyuhikari	Green	Japan	
19	Okuhikari	Green	Japan	
20	Fujiedakaori	Green	Japan	
21	Benifuuki	Black	Japan	Plucked by hand
22	Yabukita	Black	Japan	Organic
23	Benifuuki	Black	Japan	
24	Lapsang Souchong	Black	China	
25	Bainianlaoshu	Black	China	
26	Jinjunmei	Black	China	
27	Mitsukoukoucha	Black	Chinese Taipei	
28	Fbobf Extra Special New Tokutou	Black	Chinese Taipei	
29	Vithanakande Tea Factory	Black	Sri Lanka	
30	Fbobf Special New Vithanakande Tea Factory	Black	Sri Lanka	
31	Ruhunu B.O.P.I	Black	Sri Lanka	
32	A Fine Uva Tea	Black	Sri Lanka	
33	A Fine Dimbula tea	Black	Sri Lanka	
34	Rubi-Bio-Organic	Black	India	Organic
35	Puttabong	Black	India	2nd flush
36	2010 Thurbo	Black	India	2nd flush
37	Jungpana	Black	India	1st flush
38	Rohini	Black	India	2nd flush

Table S2. Volatiles determined in oolong tea (relative concentrations, bold—indentified by authentic reference material).

		Oolong tea												
		TEA 1	TEA 2	TEA 3	TEA 4	TEA 5	TEA 6	TEA 7	TEA 8	TEA 9	TEA 10	TEA 11	TEA 12	TEA 13
1	Hexanal	0	0.012507	0	0	0	0	0	0	0	0.03191	0	0	0.020512
2	Undecan	0	0	0	0	0	0	0	0	0	0	0	0	0.012185
3	Methylpentenone derivative	0	0.005117	0	0	0	0.010494	0	0	0	0	0	0	0
4	1-Penten-3-ol	0.037501	0.025021	0	0.017292	0.018767	0	0.011003	0.004343	0	0	0	0.008701	0.032568
5	unknown 1	0.039955	0.026682	0.09611	0	0	0	0	0	0	0.08007	0	0	0
6	Methylbutanol derivative	0	0	0	0.003325	0	0	0.004398	0.002038	0	0.03211	0.002753	0.005442	0
7	2-Hexenal,(E)-	0	0	0	0	0	0	0	0	0	0	0	0	0
8	**2,5-Dimethylpyrazine**	0.009007	0.009209	0.01504	0	0	0	0	0	0	0	0	0	0
9	Diexthylbenzene derivative	0	0	0	0	0	0	0	0	0.04951	0.0636	0.043865	0.053425	0.011821
10	2,5-Dimethyl pyrazine	0.009791	0.008878	0.01312	0	0	0	0	0	0	0	0	0	0
11	2-Penten-1-ol	0.011078	0.009895	0	0	0.005613	0.033937	0	0	0	0.0218	0	0.005439	0.011716
12	Benzene,1,3-diethyl-	0	0	0	0	0	0	0	0	0.003964	0.00578	0.004516	0	0
13	2-Ethyl pyrazine	0.006935	0.006448	0	0	0	0	0	0	0	0	0	0	0
14	1-Hexanol	0.003793	0.002463	0	0	0	0	0	0	0	0.06138	0	0	0.00081
15	**3-Hexen-1-ol**	0	0	0	0.004862	0	0.011102	0.008905	0	0	0.14125	0.004808	0.012967	0.017699
16	2-Hexen-1-ol, (E)-	0	0	0	0	0	0	0	0	0	0.02006	0	0	0
17	Pentylalcohol	0.002031	0.002038	0	0.004423	0.002909	0.005995	0.003713	0.001498	0.001608	0	0.001734	0.002299	0
18	**Linalool oxide I**	0.278193	0.453098	0.22692	0.360846	0.340765	0.552482	0.630453	0.277981	0.282035	1.91485	0.307824	0.427458	0.364645
19	2-Furancarboxaldehyde	0.043668	0.063263	0.12185	0	0.045555	0.03744	0	0	0	0	0	0	0
20	2,4-Heptadienal	0	0	0	0	0	0	0	0	0	0	0	0	0
21	Furan,2,5-dimethyl	0	0	0	0	0	0	0	0	0	0	0	0	0
22	**Linalool oxide II**	0.05165	0.022172	0.09671	0	0	0.027484	0.017367	0.019146	0	1.28653	0	0.0593	0.066841
23	Furan-2-propyl	0	0.005314	0	0	0	0	0	0	0	0.0155	0	0	0
24	Ethanone, 1-(2-furanyl)-	0.01129	0.014791	0.02296	0	0	0.004912	0	0	0	0	0	0	0
25	Benzenaldehyde	0	0	0	0.016045	0	0	0.002918	0.000566	0.006439	0.13214	0	0.00144	0.010979
26	**Linalool**	0.00325	0.006247	0	0.001932	0	0.009178	0.023261	0.023418	0.008339	0.10796	0.006303	0.015558	0.029783
27	2-Furancarboxaldehyde, 5-methyl-	0.024404	0.024827	0.08507	0	0.003857	0.009808	0	0	0	0	0	0	0
28	2-Heptanone, 5-methyl-	0.004989	0.0056	0	0	0	0	0	0	0	0	0	0	0
29	1H-pyrrole-2carboxaldehyde,	0.063601	0.042581	0	0	0.006086	0.060033	0.003038	0	0	0	0	0	0
30	1,5,7-Octatrien-3-ol, 3,7-dimethyl-	0.026713	0.048355	0.03544	0	0.031357	0.141985	0.014979	0.003328	0.001759	0.45281	0.007886	0.002776	0.002531
31	Benzenamine, 2-methoxy-5-methyl	0.006261	0.007924	0	0	0	0.00434	0	0	0	0	0	0	0
32	2-Furanmethanol	0.01308	0.019734	0	0	0.008345	0.0227	0	0	0	0	0	0	0
33	2(3H)-furanone, 5-ethyldihydro	0	0	0	0	0	0	0	0	0	0	0.002678	0	0
34	2(3H)-furanone, 5-ethyldihydro	0.009178	0.021197	0.01589	0.004729	0.02004	0.035016	0.020629	0.004609	0.003329	0.00515	0	0	0
35	4-Ethyl benzaldehyde	0	0	0	0.013753	0	0	0	0	0.043394	0.04822	0.042805	0.058109	0
37	Butanoic acid, 2-methyl	0	0	0	0	0	0	0	0	0	0	0	0	0
38	1-Isopropyl-2-methoxy -4-methylbenzene	0	0	0	0	0	0	0	0	0	0	0	0	0.062645

Continued

39	**Linalool oxide III**	0.038904	0.043245	0.09993	0.008465	0.016364	0.026601	0.038624	0.022874	0.011986	0.94901	0.014859	0.051462	0.051958
40	Benzenamine, 4-ethoxy-	0.004993	0.010665	0.00482	0	0	0.012728	0.020429	0.013741	0.002369	0.61736	0.003748	0.118391	0.109938
41	**Linalool oxide IV**	0.025054	0.002292	0	0	0	0.002881	0.006268	0.004644	0	0.08887	0.000547	0.002685	0.003629
42	**Methyl salicylate**	0.004201	0	0	0	0	0	0	0	0	0	0	0	0
43	**Nerol**	0	0	0	0	0	0	0	0	0	0.01623	0	0	0
44	Benzoic acid,4-ethyl, methyl ester	0	0	0	0.0047	0	0	0	0	0	0	0	0	0.083049
45	3,4-Dimethyl acetophenone	0	0	0	0.040009	0	0	0	0	0.079507	0.08847	0.078326	0.103054	0.037573
46	Benzoic acid, 4-formyl-,methylester	0	0	0	0	0	0	0	0	0	0	0	0	0
47	O-Diacetylbenzene	0	0	0	0	0	0	0	0	0	0	0	0	0
48	**Geraniol**	0.006842	0.01203	0	0	0	0.025202	0.119208	0.049504	0	0.38022	0.011039	0	0.071248
49	4-Ethyl acetophenone	0	0	0	0.033925	0	0	0	0	0.055803	0	0.053107	0.003044	0.054907
50	**Benzyl alcohol**	0.098772	0.087601	0.17541	0.066293	0.041059	0.113813	0.08896	0.036744	0.028317	1.71382	0.036558	0.044358	0.139831
51	**2-Phenylethanol**	0.144479	0.128073	0.27446	0.626597	0.368093	0.078673	0.086613	0.045294	0.160206	1.36397	0.08072	0.064703	0.154794
53	Methyl cinamate	0	0	0	0	0	0	0	0	0	0	0	0	0
54	Hexanoic acid	0	0	0	0	0	0	0	0	0	0.30249	0	0	0
55	Benzeneacetonitrile	0.048178	0.070401	0.11509	0.063322	0.056501	0.03622	0.027845	0.008752	0.078826	0	0.018449	0	0
56	**Jasmone**	0	0	0	0	0	0	0.022476	0.013458	0.005838	0	0	0.004618	0
57	Butanoic acid, 3-hexenyl ester	0	0	0	0.001616	0	0	0	0	0	0	0	0	0
58	3,7-Octadien-2, 6-diol,2,6-dimethyl-	0	0	0	0	0.002275	0	0.013942	0.005489	0	0.16256	0.002639	0.007096	0
59	Ethanone, 1-(1H-pyrrol-2-yl)-	0.065064	0.120217	0.12849	0	0.017023	0.081787	0.006378	0	0	0	0	0	0
60	4-(1-hydroxyethyl) benzaldehyde	0	0	0	0.0153	0	0	0	0	0.178687	0	0	0	0
61	4-Hydroxy-3-methylacetophenone	0	0	0	0	0	0	0	0	0	0.18045	0.191843	0.301659	0.008885
62	Phenol	0.009874	0.004779	0.0131	0	0.002407	0	0	0	0	0	0	0	0
63	1H-pyrrole-2-carboxaldehyde	0.044414	0.031137	0.13181	0	0.004833	0.020459	0	0	0	0	0	0	0
64	Furaneol	0.005049	0.00826	0	0	0	0	0	0	0	0	0	0	0
65	1,6-Octadiene-3, 5-diol,3,7-dimethyl-	0	0	0	0	0	0	0.122313	0.075155	0.029088	0.0449	0.037619	0.016984	0.018734
66	4-Hexenoic acid	0	0	0	0	0	0	0	0	0	0	0	0	0
67	Benzenemethamine	0	0.005749	0	0.032418	0	0	0	0	0	0	0	0	0
68	2-Phenylethyl benzoate	0.002601	0.010949	0	0	0.013448	0	0.005596	0.001382	0.019374	0.04077	0	0	0
69	2H-Pyran-2-one, tetrahydro-6-ethyl	0	0	0	0	0.00249	0	0.006371	0.002313	0	0	0	0	0
70	Undecanoid acid, methyl ester	0	0	0	0	0	0	0	0	0	0	0	0	0
71	**Jasmin lactone**	0.087514	0.266736	0.45832	0.150783	0.106578	0.18588	0.309478	0.145746	0.081474	0.01239	0.093367	0.020351	0.031316
72	3-Hexen-1-ol, formate,(Z)-	0	0	0	0	0	0	0	0	0	0	0	0	0
73	Methylethylmaleimide	0.012338	0.011889	0.00206	0	0	0	0.002747	0.001954	0	0.00748	0	0.001084	0
74	1H-Benzotriazole, 1-ethenyl-	0	0	0	0.491471	0	0	0	0	0.400174	0	0.01449	0	0
75	Dihydroactinidiolide	0.006033	0.010195	0	0	0	0.036396	0	0	0	0	0	0	0
76	1,7-Octadien-3, 6-diol,2,6-dimethyl-	0	0	0	0	0	0	0.008524	0	0	0.05271	0	0	0
77	**Methyl jasmonate**	0	0	0	0	0	0	0.00907	0	0	0.00168	0	0	0.001051
78	Coumaran	0.023408	0	0.03534	0	0	0.015937	0	0	0	0	0	0	0
79	**Coumarin**	0.002089	0	0	0	0	0.016262	0.013367	0.007711	0	0	0.002842	0.007176	0.001736
80	**Indole**	0	0	0.09736	0.601278	0.433303	0.240362	1.119144	0.663919	1.057987	0.01336	0.48641	0.169741	0.453921
81	Phenol, 4-propyl-	0	0	0	0	0	0	0	0	0	0	0	0	0
82	Benzaldehyde, 4-hydroxy-	0	0	0	0	0	0	0	0	0	0	0	0	0

Table S3. Volatiles determined in green tea.

		Green tea						
		TEA 14	TEA 15	TEA 16	TEA 17	TEA 18	TEA 19	TEA 20
1	Hexanal	0	0	0	0	0	0	0
2	Undecan	0	0	0	0.013286	0.011089	0.015404	0.01321
3	Methylpentenone derivative	0	0	0	0	0	0	0
4	1-Penten-3-ol	0.017191	0.011164	0	0	0	0	0.005041
5	unknown 1	0	0	0	0	0	0	0
6	Methylbutanol derivative	0.004415	0.00475	0	0.001923	0.004916	0.00629	0.004485
7	2-Hexenal,(E)-	0	0	0	0	0	0	0
8	**2,5-Dimethylpyrazine**	0	0	0	0	0	0	0
9	Diexthylbenzenederivative	0.010145	0.013787	0	0.006512	0	0.005489	0.004517
10	2,5-Dimethyl pyrazine	0	0	0	0	0	0	0
11	2-Penten-1-ol	0.005605	0	0	0	0	0	0
12	Benzene,1,3-diethyl-	0	0	0	0	0	0	0
13	2-Ethyl pyrazine	0	0	0	0	0	0	0
14	1-Hexanol	0	0	0.001165	0	0	0	0
15	**3-Hexen-1-ol**	0.006231	0.009791	0	0	0	0	0
16	2-Hexen-1-ol, (E)-	0	0	0	0	0	0	0
17	Pentylalcohol	0.001363	0.002116	0.001638	0.000603	0.001012	0.00188	0
18	**Linalool oxide I**	0.285221	0.356505	0.399367	0.361682	0.350891	0.363177	0.335858
19	2-Furancarboxaldehyde	0	0	0	0	0	0	0
20	2,4-Heptadienal	0	0	0	0	0	0	0
21	Furan,2,5-dimethyl	0	0	0	0	0	0	0
22	**Linalool oxide II**	0.001873	0.011113	0.003792	0	0	0	0
23	Furan-2-propyl	0	0	0	0	0	0	0
24	Ethanone,1-(2-furanyl)-	0	0	0	0	0	0	0
25	Benzenaldehyde	0	0.001336	0.001879	0	0	0	0
26	**Linalool**	0.003985	0.007335	0.003158	0	0	0	0.000263
27	2-Furancarboxaldehyde,5-methyl-	0	0	0	0	0	0	0
28	2-Heptanone,5-methyl-	0	0	0	0	0	0	0
29	1H-pyrrole-2carboxaldehyde,	0	0	0	0	0	0	0
30	1,5,7-Octatrien-3-ol,3,7-dimethyl-	0	0	0	0	0	0	0
31	Benzenamine,2-methoxy-5-methyl	0	0	0	0	0	0	0
32	2-Furanmethanol	0	0	0	0	0	0	0
33	2(3H)-furanone,5-ethyldihydro	0	0	0	0	0	0	0
34	2(3H)-furanone,5-ethyldihydro	0	0	0	0	0	0	0
35	4-Ethyl benzaldehyde	0.015032	0.020284	0.02492	0.012545	0.00895	0.009528	0.0097
37	Butanoic acid, 2-methyl	0	0	0	0	0	0	0
38	1-Isopropyl-2-methoxy-4-methylbenzene	0.054952	0.090987	0	0.035548	0.034376	0.023011	0.016856
39	**Linalool oxide III**	0.01598	0.005968	0.004012	0.005581	0	0.002687	0.003841

Continued

40	Benzenamine,4-ethoxy-	0	0	0	0	0	0	0
41	**Linalool oxide IV**	0	0.037983	0.026404	0.055647	0.012717	0.016636	0.02001
42	**Methyl salicylate**	0	0	0.001562	0	0	0	0
43	**Nerol**	0	0	0	0	0	0	0
44	Benzoic acid,4-ethyl, methyl ester	0.07397	0.118467	0.019743	0.053539	0.052089	0.032586	0.023506
45	3,4-Dimethyl acetophenone	0.034445	0.054957	0.050657	0.030412	0.023913	0.02371	0.020676
46	Benzoic acid,4-formyl-,methylester	0.030777	0.049499	0.010073	0.025885	0.024246	0.015527	0.009943
47	O-Diacetylbenzene	0.010382	0.018577	0	0.004793	0.004933	0	0
48	**Geraniol**	0.05234	0.074953	0.004948	0	0	0	0
49	4-Ethyl acetophenone	0.041707	0.067988	0.046961	0.03902	0.019136	0.027503	0.022749
50	**Benzyl alcohol**	0.038927	0.079246	0.021702	0.008251	0.003131	0.004859	0.004232
51	**2-Phenylethanol**	0.022699	0.045358	0.003618	0.001255	0.000744	0	0
53	Methyl cinamate	0.007159	0.011558	0	0.004382	0.004184	0	0
54	Hexanoic acid	0	0	0	0	0	0	0
55	Benzeneacetonitrile	0	0	0	0	0	0	0
56	**Jasmone**	0.005784	0.015073	0	0	0	0	0
57	Butanoic acid,3-hexenyl ester	0	0	0.001572	0	0	0	0
58	3,7-Octadien-2,6-diol,2,6-dimethyl-	0	0	0	0	0	0	0
59	Ethanone,1-(1H-pyrrol-2-yl)-	0.000823	0	0	0	0	0	0
60	4-(1-hydroxyethyl)benzaldehyde	0.013156	0.018623	0.027676	0.012013	0.009194	0.013278	0.00869
61	4-Hydroxy-3-methylacetophenone	0.01049	0.014641	0	0.008703	0.006552	0.009104	0.005837
62	Phenol	0	0	0	0	0	0	0
63	1H-pyrrole-2-carboxaldehyde	0	0	0	0	0	0	0
64	Furaneol	0	0	0	0	0	0	0
65	1,6-Octadiene-3,5-diol,3,7-dimethyl-	0	0	0	0	0	0	0
66	4-Hexenoic acid	0	0	0	0	0	0	0
67	Benzenemethamine	0	0	0	0	0	0	0
68	2-Phenylethyl benzoate	0	0	0	0	0	0	0
69	2H-Pyran-2-one,tetrahydro-6-ethyl	0	0	0	0	0	0	0
70	Undecanoid acid, methyl ester	0	0.005561	0	0.010156	0.013887	0.014884	0.008337
71	**Jasmin lactone**	0.001613	0.002837	0.007933	0	0	0	0
72	3-Hexen-1-ol,formate,(Z)-	0	0	0.013315	0	0	0	0
73	Methylethylmaleimide	0	0	0.00241	0	0	0	0
74	1H-Benzotriazole,1-ethenyl-	0	0	0	0	0	0	0
75	Dihydroactinidiolide	0	0	0.003659	0	0	0	0
76	1,7-Octadien-3,6-diol,2,6-dimethyl-	0	0	0	0	0	0	0
77	**Methyl jasmonate**	0	0	0	0	0	0	0
78	Coumaran	0	0	0.001669	0	0	0	0
79	**Coumarin**	0	0.000968	0.005591	0.018764	0.003012	0	0.003997
80	**Indole**	0.020377	0.051619	0.049513	0.002644	0.004206	0.003602	0.044296
81	Phenol, 4-propyl-	0	0	0	0	0	0	0
82	Benzaldehyde,4-hydroxy-	0	0	0.022579	0	0	0	0

Table S4. Volatiles determined in black tea.

	Black tea																	
	TEA 21	TEA 22	TEA 23	TEA 24	TEA 25	TEA 26	TEA 27	TEA 28	TEA 29	TEA 30	TEA 31	TEA 32	TEA 33	TEA 34	TEA 35	TEA 36	TEA 37	TEA 38
1 Hexanal	0.050283	0.093654	0.02275	0.019013	0.009955	0.013462	0	0.037265	0	0	0	0	0.018051	0	0	0	0	0
2 Undecan	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3 Methylpentenone derivative	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4 1-Penten-3-ol	0.221826	0.108697	0.054263	0	0.042266	0.03645	0.057938	0.117379	0.09006	0.072494	0.171505	0.076447	0.098218	0.021	0.02726	0.129086	0.084089	0.063793
5 unknown 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6 Methylbutanol derivative	0.060309	0.012216	0	0	0.027676	0.021815	0.015059	0.058327	0.02234	0.018189	0	0	0	0.011	0.041633	0.030829	0.01785	0.010756
7 2-Hexenal,(E)-	0.304533	0.102849	0	0	0	0	0	0	0	0	0	0	0.103989	0	0	0	0	0
8 **2,5-Dimethylpyrazine**	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9 Diexthylbenzene derivative	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10 2,5-Dimethyl pyrazine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11 2-Penten-1-ol	0.349069	0.067658	0.024233	0.016819	0.03806	0.022797	0.067319	0.095468	0.068516	0.071106	0.106472	0.034418	0.049442	0.0155	0.018473	0.094426	0.0578	0.03536
12 Benzene,1, 3-diethyl-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13 2-Ethyl pyrazine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14 1-Hexanol	0.056901	0.036568	0	0.011389	0.027039	0.014769	0.01231	0.038591	0.055546	0.05197	0.052052	0.017145	0.022088	0.0219	0.038706	0.106503	0.051764	0.036871
15 **3-Hexen-1-ol**	0.68145	0.170899	0.019385	0.053407	0.144201	0.063563	0.085587	0.281916	0.140618	0.125208	0.243671	0.108932	0.120272	0.1868	0.173864	0.545573	0.191814	0.135573
16 2-Hexen-1-ol, (E)-	0.086734	0.050134	0	0	0.026137	0.012984	0.017542	0.102118	0.125691	0.088498	0.136779	0.027993	0.039083	0.0322	0.012939	0.227329	0.067095	0.099996
17 Pentylalcohol	0	0	0	0	0	0.003327	0.00361	0.003237	0.001981	0	0.008257	0.004993	0.004286	0.0057	0.004501	0.004907	0.005546	0.006962
18 **Linalool oxide I**	1.421303	0.908019	0.52101	0.441741	0.542082	0.508451	0.735071	1.233934	0.359785	0.38176	0.91989	0.48981	0.526897	0.5464	0.897974	1.88714	0.783807	0.729617
19 2-Furancarboxaldehyde	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0167	0	0	0	0
20 2,4-Heptadienal	0	0.039495	0.015084	0	0	0	0	0.00757	0	0	0	0.005969	0.025793	0	0	0	0	0
21 Furan,2,5-dimethyl	0	0	0	0.024266	0	0	0	0	0	0	0	0	0	0	0	0.029264	0	0.011259
22 **Linalool oxide II**	1.013935	0.336041	0.080694	0.191938	0.460204	0.373073	0.39009	0.954359	0.056171	0.043468	0.255203	0.162615	0.159972	0.341	0.903061	2.002691	0.84779	0.460012
23 Furan-2-propyl	0	0.020668	0.005399	0.00417	0	0	0	0.006767	0	0	0	0.00592	0.014718	0	0.002775	0.010959	0.004107	0.006941
24 Ethanone, 1-(2-furanyl)-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25 Benzenaldehyde	0.052889	0.176659	0.011528	0.033005	0.018196	0.01962	0.045454	0.074875	0.005205	0.004967	0.03405	0.012672	0.020547	0.0115	0.052299	0.048453	0.026628	0.020711
26 **Linalool**	0.183418	0.061673	0.013959	0.012666	0.395096	0.213822	0.440133	0.0957	0.149427	0.106838	0.261172	0.135233	0.069957	0.158	0.21579	0.625765	0.279275	0.076368
27 2-Furancarboxaldehyde, 5-methyl-	0	0	0	0.009288	0	0	0	0	0	0	0	0	0	0	0	0.009857	0	0.00267
28 2-Heptanone,5-methyl-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29 1H-pyrrole-2carboxaldehyde,	0	0	0	0	0.01197	0.020797	0	0	0	0	0	0	0	0	0	0.018912	0	0
30 1,5,7-Octatrien-3-ol,3, 7-dimethyl-	0.25257	0.015052	0.02273	0.017818	0.023619	0.043578	0.083637	0.262481	0	0	0.001884	0	0	0.0136	0.005206	0.192591	0.043988	0.018029
31 Benzenamine, 2-methoxy-5-methyl	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32 2-Furanmethanol	0.005845	0	0	0.024004	0	0.013261	0.007284	0	0	0	0.008218	0	0	0.0077	0	0.032194	0	0.01831
33 2(3H)-furanone, 5-ethyldihydro	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.024685	0.027189	0	0
34 2(3H)-furanone, 5-ethyldihydro	0.221295	0.017553	0.014349	0.009645	0	0	0	0	0	0	0	0	0.008058	0	0	0	0	0
35 4-Ethyl benzaldehyde	0.003557	0	0	0	0	0	0	0	0	0	0	0	0.006924	0	0.015621	0.009966	0.017499	0.024888
37 Butanoic acid, 2-methyl	0	0	0	0	0.015269	0.010993	0	0	0	0	0	0	0	0	0	0	0	0
38 1-Isopropyl-2-methoxy -4-methylbenzene	0	0.010727	0	0.024325	0	0	0	0	0	0.003718	0	0	0.013112	0.0133	0.034859	0.030887	0	0
39 **Linalool oxide III**	0.27328	0.227825	0.064895	0.007336	0.133178	0.120907	0.203789	0.45679	0.003523	0.00301	0.020806	0.00877	0.015719	0.0282	0.107531	0.151916	0.112499	0.055263
40 Benzenamine, 4-ethoxy-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Continued

41	**Linalool oxide IV**	0.400065	0.314051	0.09242	0.234096	0.377233	0.371979	0.338915	0.389507	0.013419	0.012608	0.09257	0.052481	0.065295	0.1057	0.361725	0.417372	0.274188	0.14112
42	**Methyl salicylate**	0.341064	0.008798	0.005093	0.006317	0.035978	0.035617	0.344129	0.038024	0.033946	0.022326	0.085551	0.213584	0.070652	0.0452	0.074226	0.280135	0.078688	0.070898
43	**Nerol**	0.007634	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	Benzoic acid,4-ethyl, methyl ester	0.034652	0.018349	0.010655	0.036014	0.016726	0.018068	0.01528	0.021509	0.00278	0.005191	0.020954	0.009456	0.022513	0.0127	0.02655	0.039468	0.008323	0.013059
45	3,4-Dimethyl acetophenone	0.034671	0.014419	0.010484	0.019022	0.018986	0.013704	0.013407	0.015588	0.009241	0.012663	0.024304	0.011816	0.027815	0.0138	0.042523	0.044568	0.036923	0.056455
46	Benzoic acid,4-formyl-, methylester	0.01268	0.006884	0	0.023985	0.006635	0.007701	0.006375	0.010466	0	0	0.009514	0.004802	0.009317	0.4446	0.010626	0.016358	0	0.006815
47	O-Diacetylbenzene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	**Geraniol**	1.260518	0.043723	0.035917	0.100754	0.756134	0.846676	0.048052	0.392736	0	0	0.030293	0.014303	0.008994	0	0.476999	0.661557	0.204581	0.245601
49	4-Ethyl acetophenone	0.030387	0.016643	0.010363	0	0.020332	0.012543	0.012889	0.017052	0.007192	0.011467	0.023453	0.01187	0.024516	0.0141	0.034743	0.042477	0.033361	0.048638
50	**Benzyl alcohol**	1.210593	1.47216	0.233963	0.734092	0.47722	0.56876	0.576994	1.173924	0.101389	0.080222	0.15104	0.050872	0.126068	0.1284	0.344552	0.502736	0.259551	0.392265
51	**2-Phenylethanol**	1.997018	1.096002	0.327	0.610552	1.678485	1.256742	0.276295	0.936773	0.177187	0.143328	0.202683	0.038435	0.055666	0.1268	0.414552	0.609475	0.281816	0.193228
53	Methyl cinamate	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	Hexanoic acid	0.255744	1.481868	0	0	0.145494	0.120495	0.036914	0.085249	0	0	0.258387	0.187449	0.086971	0	0.157828	0.208848	0.123217	0
55	Benzeneacetonitrile	0	0.051786	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	**Jasmone**	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	Butanoic acid, 3-hexenyl ester	0.047871	0.028818	0.01865	0	0	0	0.01376	0.03272	0	0	0	0	0	0	0	0	0	0
58	3,7-Octadien-2,6-diol, 2,6-dimethyl-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	Ethanone, 1-(1H-pyrrol-2-yl)-	0.035699	0	0.00802	0.055288	0.02063	0.037997	0.012331	0.009871	0	0	0.035819	0	0	0.0318	0.024081	0.084593	0.016088	0.034741
60	4-(1-hydroxyethyl) benzaldehyde	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	4-Hydroxy-3-methylacetophenone	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	Phenol	0	0	0	0	0	0.00397	0.006189	0	0	0	0	0	0	0	0	0	0	0
63	1H-pyrrole-2 -carboxaldehyde	0.008994	0	0	0.084289	0.013804	0.036317	0.012636	0.008509	0	0	0.003622	0	0	0.0138	0.027124	0.02584	0.003969	0.011776
64	Furaneol	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.017884	0	0
65	1,6-Octadiene-3, 5-diol,3,7-dimethyl-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	4-Hexenoic acid	2.204504	0.223613	0.394017	0	0.566074	0	0.182465	0	0	0	0	0	0	1.1489	1.450741	1.308687	0	0.579922
67	Benzenemethamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	2-Phenylethyl benzoate	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69	2H-Pyran-2-one, tetrahydro-6-ethyl	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	Undecanoid acid, methyl ester	0.043795	0.029795	0.016643	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	**Jasmin lactone**	0	0.009082	0.003701	0.005857	0	0	0	0	0	0	0	0	0	0	0	0.006491	0	0
72	3-Hexen-1-ol, formate,(Z)-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
73	Methylethylmaleimide	0	0	0	0	0	0	0	0	0	0	0	0	0.005608	0	0	0	0	0
74	1H-Benzotriazole, 1-ethenyl-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75	Dihydroactinidiolide	0	0	0.008384	0	0	0	0	0	0	0	0	0.008396	0.015198	0	0.015543	0	0	0
76	1,7-Octadien-3, 6-diol,2,6-dimethyl-	0	0.01333	0	0	0	0	0.000585	0	0	0	0	0	0	0	0	0	0	0
77	**Methyl jasmonate**	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
78	Coumaran	0	0	0.002577	0.004031	0.002005	0.004051	0.004994	0.00267	0	0	0	0	0	0.0091	0.004341	0.018345	0	0.006257
79	**Coumarin**	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.040482	0	0
80	**Indole**	0	0.012561	0.001285	0	0	0	0	0	0	0	0	0	0.001363	0	0	0	0	0
81	Phenol, 4-propyl-	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0136	0.01508	0	0	0
82	Benzaldehyde, 4-hydroxy-	0	0	0.019254	0.021435	0	0	0	0	0	0	0	0	0	0	0.060349	0	0	0