Supplementary Materials

Table S1. Classification standard for soil fertility

Index	Different levels		
	I	II	III
pH value	5.0 ~ 5.5	4.5 ~ 5.0	< 4.5
Organic matter content (g/kg)	> 15	10 ~ 15	< 10
Cation Exchange Capacity (mmoL/kg)	> 20	15 ~ 20	< 15
Total nitrogen (g/kg)	> 1.0	0.8 ~ 1.0	< 0.8
Total phosphorus (g/kg)	> 0.6	0.4 ~ 0.6	< 0.4
Total potassium (g/kg)	> 10	5 ~ 10	< 5
Available nitrogen (mg/kg)	> 100	50 ~ 100	< 50
Available phosphorus (mg/kg)	> 10	5 ~ 10	< 5
Available potassium (mg/kg)	> 120	80 ~ 120	< 80

Note: I: The soil has good fertility; II: Soil fertility is moderate; III: The soil fertility is poor;

Reference:

1. Ministry of Agriculture and Rural Affairs of the People's Republic of China. NY/T 853-2004 Environmental requirement for growing area of tea [M]. China Standards Press, Beijing. **2015**, pp. 1–7
2. Mehra, A.; Baker, C.L. Leaching and bioavailability of aluminium, copper and manganese from tea (*Camellia sinensis*). *Food Chem.* **2017**, *100*, 1456–1463. https://doi.org/10.1016/j.foodchem.2005.11.038.
3. Mohammad, N.; Samar, M.; Alireza, I. Levels of Cu, Zn, Pb and Cd in the leaves of the tea plant (*Camellia sinensis*) and in the soil of Gilan and Mazandaran farms of Iran. *Food Meas.* **2014**, *8*, 277–282. https://doi.org/10.1007/s11694-014-9186-3.

Table S2. Aroma threshold and odor characteristics of some aroma compounds

Compound	Threshold value* μg/kg	Splits of odor characteristic (%)**					
		Woody	Floral	Burnt	Green	Fruity	Fatty
1-Octen-3-ol	0.04	0	0	80	10	0	10
3,5-Octadien-2-one	0.15	0	0	100	0	0	0
D-Limonene	0.038	10	0	0	20	70	0
α-Ionone	0.007	15	85	0	0	0	0
β-Cyclocitral	0.003	10	0	0	20	70	0
β- Ionone	0.0075	50	30	20	0	0	0
Benzaldehyde	3.5	5	0	0	10	75	10
trans-Nerolidol	0.015	0	85	0	15	0	0
Benzaldehyde, 4-methyl-	3.5	5	0	0	10	75	10
trans-Nerolidol	0.015	0	85	0	15	0	0
Linalool	0.5	0	100	0	0	0	0
2,4-Heptadienal, (E,E)-	0.49	0	0	0	0	0	100
Furfural	0.282	0	0	80	0	0	20
Citral	0.032	10	0	0	20	70	0
Methyl salicylate	0.04	0	70	30	0	0	0
2-Penten-1-ol, (Z)-	0.4	0	0	0	100	0	0
Geranylacetone	0.186	0	90	0	0	0	10
Geraniol	0.0032	0	100	0	0	0	0
Myrcene	13	50	20			30	
Ionone oxide	0.007	50	30	20	0	0	0
s-Triazolo[1,5-a]pyridine, 2,5,7-trimethyl-	0.282	0	0	80	0	0	20

* Threshold Values were referred to Van et al (1,2).

** Splits of odor characteristics were referred to Lin (3).

1. Van, G.L.J. Compilations of flavor threshold values in water and other media; Boelens Aroma Chemical Information Services: Houten, The Netherlands. 2003.
2. Van, G.L.J. Compilations of odour threshold values in air, water and other media; Second enlarged and revised edition; Boelens Aroma Chemical Information Services: Houten, The Netherlands. 2011.
3. Lin, X.Y. Perfumery, 3rd ed.; Chemical Industry Press: Beijing, China. 2018.

Table S3. GC-MS analysis of volatile compounds in tea leaves planted in soils with different pH

Compound	pH 5.32 (μg/kg)	pH 4.74 (μg/kg)	pH 4.13 (μg/kg)	pH 3.29 (μg/kg)
Terpenoids				
1,3-Cyclohexadiene, 1,5,5,6-tetramethyl-	0.173±0.023	0	0	0
2,6-Dimethyl-2-trans-6-octadiene	1.094±0.145	0.450±0.029	0.062±0.008	0
Cyclopropanecarboxylic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester	0.255±0.031	0.125±0.038	0	0
Allo-Ocimene	1.381±0.164	0.343±0.029	0.088±0.011	0
D-Limonene	0.731±0.051	1.295±0.053	0.118±0.024	0.432±0.021
α-Bulnesene	0.040±0.008	0.040±0.009	0.096±0.009	0
α-Terpinene	0.186±0.014	0.246±0.035	0	0
α-Terpinolene	0.468±0.025	0.330±0.027	0.629±0.042	0
α-Ionone	2.184±0.122	1.862±0.091	1.592±0.085	1.197±0.136
β-Cyclocitral	0.595±0.082	0.522±0.052	0.206±0.023	0.444±0.038
β- Ionone	3.092±0.161	2.202±0.114	2.149±0.112	1.242±0.137
β-Ionon-5,6-epoxide	0.126±0022	0.177±0.026	0.377±0.013	0.168±0.023
γ-Terpinene	0.262±0.018	0.123±0.035	0	0
Menthalactone	0.098±0.019	0.068±0.012	0	0.068±0.018
4-Oxoisophorone	0	0	0	0.178±0.014
trans-Nerolidol	0.045±0.011	0.043±0.012	0.046±0.014	0.117±0.017
Dihydroactindiolide	0.143±0.021	0.180±0.016	0.599±0.058	0.310±0.006
(E)-ψ-Ionone	0	0.070±0.011	0.115±0.027	0.097±0.012
Linalool	11.251±0.462	8.448±0.281	5.390±0.293	2.480±0.205
(E,E)--Farnesal	0.048±0.009	0.055±0.011	0.083±0.010	0.034±0.006
β-Ocimene	0.873±0.017	0.560±0.041	0	0
Ocimene mixture	0	0	0	0.090±0.013
Citral	0	0	0	0.249±0.026
Pinane, endo	0.927±0.027	1.182±0.032	1.212±0.125	0.560±0.016
α-Terpineol	0.078±0.011	0	0	0.064±0.013
Geraniol	11.274±0.392	8.266±0.234	5.326±0.387	3.390±0.238
Geranylacetone	2.990±0.123	1.351±0.092	0.841±0.025	0.518±0.031
Carvenone	0.204±0.013	0.295±0.024	0.544±0.064	0.209±0.028
Isophytol	0.053±0.008	0.146±0.018	0.172±0.021	0.053±0.007
Myrcene	0.412±0.014	0.493±0.032	0	0.116±0.013
Phytol	0.257±0.022	0.320±0.024	0.365±0.034	0.051±0.008
Phytone	0.176±0.016	0.261±0.018	0.536±0.037	0.065±0.010
Hydrocarbons				
o-Xylene	1.661±0.158	1.830±0.084	0.573±0.024	0.253±0.014
Naphthalene, 1,2,3,4-tetrahydro-1,6,8-trimethyl-	0.320±0.013	0.290±0.021	0.123±0.016	0.136±0.019
Benzene, 1,2,3,5-tetramethyl-	0.158±0.013	0.125±0.021	0	0
Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	0.029±0.007	0.054±0.009	0.071±0.011	0
Benzene, 1,2,4-trimethyl-	0	0.402±0.023	0	0.138±0.017
Benzene, 2-(2-butenyl)-1,3,5-trimethyl-	0.067±0.006	0	0	0
Naphthalene, 2,6-dimethyl-	0.252±0.011	0.184±0.015	0.341±0.034	0

Benzene, 4-(2-butenyl)-1,2-dimethyl-, (E)-	0.168±0.012	0	0	0
Benzaldehyde, 4-methyl-	0	0	0	0.130±0.08
Paroxypropione	0	0	0	0.108±0.016
p-Cymene	1.230±0.021	0	0	0
Benzene, 1-ethyl-4-methyl-	0	0	0	0.148±0.012
m-Cymene	0	0.116±0.021	0	0
o-Cymene	0.387±0.018	0.544±0.018	0.209±0.025	0.324±0.018
o-Isopropenyltoluene	0.317±0.013	0.198±0.022	0.080±0.007	0.138±0.012
Benzaldehyde, 2-hydroxy-	0.246±0.012	0.137±0.019	0.143±0.012	0.041±0.008
1, 1, 5-Trimethyl-1, 2-dihydronaphthalene	2.787±0.185	1.693±0.143	1.483±0.203	1.060±0.052
Heterocycles				
1H-Pyrrole, 1-ethyl-	1.136±0.124	0.411±0.036	0	0
1H-Pyrrole, 1-(2-furanylmethyl)-	0.391±0.012	0.241±0.029	0	0
trans-2-(2-Pentenyl)furan	0.102±0.011	0	0	0
Benzofuran, 2,3-dihydro-	0.142±0.014	0.121±0.014	0.092±0.008	0
1H-Pyrrole-3-carboxylic acid, 2,4-dimethyl-, methyl ester	0.201±0.013	0	0	0
Pyrazine, 3,5-diethyl-2-methyl-	0.131±0.009	0.107±0.017	0	0
Furan, 2-ethyl-5-methyl-	0.312±0.015	0.240±0.024	0.129±0.014	0.106±0.014
Ethanone, 1-(1H-pyrrol-2-yl)-	0.399±0.016	0.418±0.013	0.399±0.013	0.230±0.016
Ethanone, 1-(2-furanyl)-	0.587±0.018	0	0	0
2-n-Butyl furan	1.003±0.106	0	0	0
Nicotinyl alcohol	0.067±0.008	0.077±0.012	0.063±0.006	0
1H-Indole, 3-methyl-	0.063±0.011	0.083±0.011	0.082±0.009	0
4,5-Diamino-6-hydroxypyrimidine	0.130±0.014	0	0	0
2-Furancarboxaldehyde, 5-methyl-	0.621±0.018	1.106±0.018	0.941±0.037	0.662±0.074
6-Quinazolinol	0	0.051±0.013	0.058±0.009	0
1H-Pyrrole-2-carboxaldehyde	0.160±0.011	0.122±0.021	0.131±0.026	0.079±0.011
1H-Pyrrole-2-carboxaldehyde, 1-ethyl-	2.167±0.157	2.170±0.014	1.539±0.218	1.099±0.068
Indole	0.050±0.009	0.099±0.011	0	0
s-Triazolo[1,5-a]pyridine, 2,5,7-trimethyl-	0.166±0.012	0	0	0
Carbazole, 2,5-dimethyl-	0	0.046±0.009	0.049±0.011	0
Alcohols				
2-Penten-1-ol, (Z)-	0	0.135±0.015	0	0.110±0.08
1-Octen-3-ol	0.151±0.024	0.644±0.046	0	0
2-Pentadecanol	0.373±0.013	0	0	0
Ketones				
5-Hepten-2-one, 6-methyl-	0.289±0.011	0.482±0.042	0.330±0.018	1.279±0.164
6,8-Nonadien-2-one, 6-methyl-5-(1-methylethylidene)-	0.408±0.014	0.315±0.039	0	0
3,5-Octadien-2-one	0	0	0	0.101±0.017
6-Methyl-3,5-heptadiene-2-one	0	0.120±0.013	0	0.457±0.013
2-Cyclopenten-1-one, 2-methyl-	0	0	0.062±0.016	0.065±0.009
Ethanone, 1-(2-methylphenyl)-	0.356±0.009	0.354±0.041	0.495±0.044	0.259±0.014
Aldehydes				

5-Heptenal, 2,6-dimethyl-	0.198±0.005	0.144±0.019	0.159±0.184	0
Furfural	0.618±0.053	1.087±0.057	1.246±0.109	1.629±0.213
2,4-Heptadienal, (E,E)-	0.105±0.008	0.176±0.016	0.085±0.011	0.268±0.038
Benzaldehyde	0.371±0.011	0.678±0.024	0	1.137±0.217
Benzaldehyde, 3-ethyl-	0.060±0.010	0.086±0.011	0.210±0.017	0.141±0.016
Benzaldehyde, 2,4,5-trimethyl-	0.171±0.013	0.230±0.041	0.286±0.021	0.236±0.015
Esters				
Hexanoic acid, 3-hexenyl ester, (Z)-	0.348±0.014	0.082±0.013	0	0
Hexadecanoic acid, methyl ester	0.084±0.009	0.085±0.008	0.118±0.015	0.035±0.009
Sulfurous acid, dimethyl ester	0	0.128±0.015	0	0
3-Phenylpropionic acid. 3,5-difluorophenyl ester	0.331±0.012	0.326±0.027	0.453±0.024	0.347±0.018
Methyl salicylate	1.355±0.075	0.848±0.024	0.645±0.049	0.118±0.031
Total	**60.084**	**46.238**	**31.142**	**22.966**

Table S4. Analysis of odor activity values (OAV) and their odor characteristics of key compounds in tea leaves at a soil pH of 3.29

Compound	Ci (μg/kg)	OAVi	%	OAV-Splitting of Odor Characteristic					
				Woody	Floral	Burnt	Green	Fruity	Fatty
D-Limonene	0.432±0.021	11.37±0.55	0.70	1.14±0.06	0	0	2.27±0.11	7.96±0.39	0
α-Ionone	1.197±0.136	171.07±19.43	10.60	25.66±2.91	145.41±16.51	0	0	0	0
β-Cyclocitral	0.444±0.038	148.00±12.67	9.17	14.80±1.27	0	0	29.60±2.53	103.60±8.87	0
β- Ionone	1.242±0.137	165.66±18.27	10.27	82.83±9.13	49.70±5.48	33.13±3.65	0	0	0
β-Ionon-5,6-epoxide	0.168±0.023	23.96±3.29	1.49	11.98±1.64	7.19±0.99	4.79±0.66	0	0	0
trans-Nerolidol	0.117±0.017	7.77±1.13	0.48	0	6.61±0.96	0	1.17±0.17	0	0
Linalool	2.480±0.205	4.96±0.41	0.31	0	4.96±0.41	0	0	0	0
Citral	0.249±0.026	7.77±0.81	0.48	0.78±0.08	0	0	1.55±0.16	5.44±0.57	0
Geraniol	3.390±0.238	1059.38±74.38	65.66	0	1059.38±74.38	0	0	0	0
Geranylacetone	0.518±0.031	2.78±0.17	0.17	0	2.51±0.15	0	0	0	0.28±0.02
1-Octen-3-ol	0	0	0	0	0	0	0	0	0
Furfural	1.629±0.213	5.78±0.76	0.36	0	0	4.62±0.60	0	0	1.16±0.15
Methyl salicylate	0.118±0.031	2.96±0.77	0.18	0	2.07±0.54	0.89±0.23	0	0	0
Total	11.984	1611.45		137.19	1277.81	43.43	34.59	116.99	1.43
%**				8.51	79.30	2.70	2.15	7.26	0.09

Note: The OAV values of volatile compounds were calculated as OAVi = Ci/Ti, where OAVi is the OAV value of compound i, Ci is the content of compound i (μg/kg), and Ti is the threshold value of compound i (μg/kg). The total OAV value (OVAt) of tea compounds was the sum of OAVi values of aroma active compounds, that is, OVAt = ∑OAVi. %** is proportion of the each odor OAV accounting for OAVt.

Table S5. Analysis of odor activity values (OAV) and their odor characteristics of key compounds in tea leaves at a soil pH of 4.13

Compound	Ci (μg/kg)	OAVi	%	OAV-Splitting of Odor Characteristic					
				Woody	Floral	Burnt	Green	Fruity	Fatty
D-Limonene	0.118±0.024	3.12±0.63	0.13	0.31±0.06	0	0	0.62±0.13	2.18±0.44	0
α-Ionone	1.592±0.085	227.39±12.14	9.70	34.11±1.82	193.28±10.32	0	0	0	0
β-Cyclocitral	0.206±0.023	68.67±7.67	2.93	6.87±0.77	0	0	13.73±1.53	48.07±5.37	0
β- Ionone	2.149±0.112	286.48± 14.93	12.21	143.24±7.47	85.94±4.48	57.30±2.99	0	0	0
β-Ionon-5,6-epoxide	0.377±0.013	53.80±1.86	2.29	26.90±0.93	16.14±0.56	10.760±0.37	0	0	0
trans-Nerolidol	0.046±0.014	3.07±0.93	0.13	0	2.61±0.79	0	0.46±0.14	0	0
Linalool	5.390±0.293	10.78±0.59	0.46	0	10.78±0.59	0	0	0	0
Citral	0	0	0	0	0	0	0	0	0
Geraniol	5.326±0.387	1664.53±120.94	70.80	0	1664.53±120.94	0	0	0	0
Geranylacetone	0.841±0.025	4.52±0.13	0.19	0	4.07±0.12	0	0	0	0.45±0.01
1-Octen-3-ol	0	0	0	0	0	0	0	0	0
Furfural	1.246±0.184	4.42±0.65	0.19	0	0	3.54±0.52	0	0	0.88±0.13
Methyl salicylate	0.645±0.049	16.13±1.22	0.68	0	11.29±0.86	4.84±0.37	0	0	0
Total	17.935	2342.90		211.43	1988.64	76.43	14.82	50.25	1.34
**%				9.024	84.880	3.262	0.632	2.145	0.057

Note: The OAV values of volatile compounds were calculated as OAVi = Ci/Ti, where OAVi is the OAV value of compound i, Ci is the content of compound i (μg/kg), and Ti is the threshold value of compound i (μg/kg). The total OAV value (OVAt) of tea compounds was the sum of OAVi values of aroma active compounds, that is, OVAt = ∑OAVi. %** is proportion of the each odor OAV accounting for OAVt.

Table S6. Analysis of odor activity values (OAV) and their odor characteristics of key compounds in tea leaves at a soil pH of 4.74

Compound	Ci (μg/kg)	OAVi	%	OAV-Splitting of Odor Characteristic					
				Woody	Floral	Burnt	Green	Fruity	Fatty
D-Limonene	1.295±0.053	34.08±1.39	0.99	3.41±0.14	0	0	6.82±0.28	23.86±0.98	0
α-Ionone	1.862±0.091	265.95±13.00	7.72	39.89±1.95	226.06±11.05	0	0	0	0
β-Cyclocitral	0.522±0.052	174.16±17.33	5.05	17.42±1.73	0	0	34.83±3.47	121.91±12.13	0
β- Ionone	2.202±0.114	293.65±15.20	8.52	146.82±7.60	88.09±4.56	58.73±3.04	0	0	0
β-Ionon-5,6-epoxide	0.177±0.026	25.35±3.71	0.74	12.68±1.86	7.61±1.11	5.07±0.74	0	0	0
trans-Nerolidol	0.043±0.012	2.88±0.80	0.08	0	2.45±0.68	0	0.43±0.12	0	0
Linalool	8.448±0.281	16.90±0.56	0.49	0	16.90±0.56	0	0	0	0
Citral	0	0	0	0	0	0	0	0	0
Geraniol	8.266±0.234	2583.14±73.12	74.97	0	2583.14±73.12	0	0	0	0
Geranylacetone	1.351±0.092	7.27±0.49	0.21	0	6.54±0.45	0	0	0	0.73±0.05
1-Octen-3-ol	0.644±0.046	16.11±1.15	0.47	0	0	12.89±0.92	1.61±0.12	0	1.61±0.012
Furfural	1.087±0.057	3.86±0.20	0.11	0	0	3.08±0.16	0	0	0.77±0.04
Methyl salicylate	0.848±0.024	21.20±0.60	0.62	0	14.84±0.42	6.36±0.18	0	0	0
Total	28.228	3445.46		220.25	2945.62	86.13	43.69	145.77	3.11
**%				6.39	85.49	2.50	1.27	4.23	0.09

Note: The OAV values of volatile compounds were calculated as OAVi = Ci/Ti, where OAVi is the OAV value of compound i, Ci is the content of compound i (μg/kg), and Ti is the threshold value of compound i (μg/kg). The total OAV value (OVAt) of tea compounds was the sum of OAVi values of aroma active compounds, that is, OVAt = ∑OAVi. %** is proportion of the each odor OAV accounting for OAVt.

Table S7. Analysis of odor activity values (OAV) and their odor characteristics of key compounds in tea leaves at a soil pH of 5.32

Compound	Ci (μg/kg)	OAVi	%	OAV-Splitting of Odor Characteristic					
				Woody	Floral	Burnt	Green	Fruity	Fatty
D-Limonene	0.731±0.051	19.25±1.34	0.42	1.92±0.13	0	0	3.85±0.27	13.47±0.94	0
α-Ionone	2.183±0.122	311.88±17.43	6.83	46.78±2.61	265.10±14.81	0	0	0	0
β-Cyclocitral	0.594±0.082	198.09±27.33	4.34	19.81±2.73	0	0	39.62±5.47	138.66±19.13	0
β- Ionone	3.092±0.161	412.22±21.33	9.03	206.11±10.67	123.67±6.40	82.44±4.27	0	0	0
β-Ionon-5,6-epoxide	0.126±0.022	17.93±3.14	0.39	8.96 ±1.57	5.38±0.94	3.59±063	0	0	0
trans-Nerolidol	0.045±0.011	2.97±0.73	0.07	0	2.52± 0.62	0	0.45±0.11	0	0
Linalool	11.251±0.462	22.50±0.92	0.49	0	22.50±0.92	0	0	0	0
Citral	0	0	0	0	0	0	0	0	0
Geraniol	11.274±0.392	3523.06±122.50	77.18	0	3523.06±122.50	0	0	0	0
Geranylacetone	2.990±0.123	16.08±0.66	0.35	0	14.47±0.60	0	0	0	1.61±0.07
1-Octen-3-ol	0.151±0.024	3.78±0.60	0.08	0	0	3.02±0.48	0.38±0.06	0	0.38± 0.06
Furfural	0.618±0.053	2.19±0.19	0.05	0	0	1.75±0.15	0	0	0.44±0.04
Methyl salicylate	1.355±0.075	33.87±1.88	0.74	0	23.71±1.31	10.16±0.56	0	0	0
Total	34.410	4563.82		283.59	3980.41	100.96	44.29	152.14	2.42
**%				6.21	87.22	2.21	0.97	3.33	0.05

Note: The OAV values of volatile compounds were calculated as OAVi = Ci/Ti, where OAVi is the OAV value of compound i, Ci is the content of compound i (μg/kg), and Ti is the threshold value of compound i (μg/kg). The total OAV value (OVAt) of tea compounds was the sum of OAVi values of aroma active compounds, that is, OVAt = ∑OAVi. %** is proportion of the each odor OAV accounting for OAVt.