

Quality Differences of Longnan Green Tea Based on Physicochemical Parameters and Volatile Organic Compound Profile

by

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Supplementary Materials

Table S1. Information about the Longnan green tea used in this study. **Table S2.** Headspace gas chromatography-ion mobility spectrometry (HS-GC-IMS) profiling of volatile organic compounds (VOCs) of Longnan green tea from different counties (Wenxian, WX; Wudu, WD; Kangxian, KX): Chromatographic and spectral data, relative content and aroma characteristics.

Table S1. Information about the Longnan green tea used in this study.

Green tea code	Green tea name	Origin area	
		Town	County
WX-1	Longjing 43	Zhongmiao	Wenxian
WX-2	Mao Feng	Zhongmiao	Wenxian
WX-3	Longjing 43	Bikou	Wenxian
WX-4	Zhongnong 108	Bikou	Wenxian
WX-5	Ze Chun Yu Ye	Bikou	Wenxian
WX-6	Premium Show Buds	Bikou	Wenxian
WX-7	Grade II Show Buds	Bikou	Wenxian
WX-8	Zi Zhu	Bikou	Wenxian
WD-1	Longjing	Yuhe	Wudu
WD-2	Mao feng	Yuhe	Wudu
WD-3	Longjing	Yuhe	Wudu
WD-4	Mao Feng	Yuhe	Wudu
WD-5	Yueqing-Wu Niu Zao	Yuhe	Wudu
WD-6	Yuyu-Bird's Tongue	Yuhe	Wudu
WD-7	Mao Jian	Yuhe	Wudu
KX-1	Premium Cuizhu	Yangba	Kangxian
KX-2	Boutique Longjing	Yangba	Kangxian
KX-3	Premium Cuifeng	Yangba	Kangxian
KX-4	Premium Cuifeng	Yangba	Kangxian
KX-5	Premium Cuifeng	Yangba	Kangxian
KX-6	Premium Cuifeng	Yangba	Kangxian
KX-7	Premium Cuifeng	Yangba	Kangxian
KX-8	Premium Cuizhu	Yangba	Kangxian
KX-9	Premium Cuifeng	Yangba	Kangxian

1 Table S2. Headspace gas chromatography-ion mobility spectrometry (HS-GC-IMS) profiling of volatile organic compounds (VOCs) of Longnan green tea from different counties
 2 (Wenxian, WX; Wudu, WD; Kangxian, KX): Chromatographic and spectral data, relative content and aroma characteristics.

No.	CAS	Compound name	RI	Rt (min)	Dt (ms)	Relative content (%)			Aroma characteristic
						WX	WD	KX	
1	123-38-6	Propanal	481.5	2.24	1.036	4.45±0.97 ^b	5.52±1.05 ^{ab}	6.71±1.63 ^a	Floral, pungent, solvent
2	67-63-0	2-Propanol	493.3	2.33	1.078	0.72±0.16 ^a	0.79±0.15 ^a	0.37±0.21 ^b	Floral
3	141-78-6	Ethanol D	499.5	2.38	1.126	3.43±1.54 ^a	4.48±0.92 ^a	1.01±1.29 ^b	/
		Ethanol	501.9	2.40	1.051	3.56±0.59 ^a	3.34±0.82 ^a	3.70±1.05 ^a	
4	109-94-4	Ethyl formate	508	2.45	1.082	0.35±0.05 ^a	0.39±0.04 ^a	0.36±0.05 ^a	Pungent
5	67-64-1	Acetone	513.2	2.50	1.118	7.20±0.62 ^b	6.86±0.47 ^b	9.21±1.23 ^a	
6	67-64-1	2-Propanone	529.1	2.63	1.127	0.58±0.13 ^a	0.56±0.27 ^a	0.43±0.08 ^b	
7	79-20-9	Methyl acetate D	533.5	2.67	1.198	1.71±1.89 ^b	4.06±2.34 ^a	1.50±0.76 ^b	Ester, green
		Methyl acetate	539.3	2.73	1.035	1.34±0.39 ^b	1.69±0.44 ^{ab}	2.10±0.57 ^a	
8	71-23-8	1-Propanol D	552.2	2.85	1.249	0.82±0.50 ^b	1.14±0.56 ^a	0.41±0.17 ^b	Alcohol, candy, pungent
		1-Propanol	553.7	2.86	1.105	1.90±0.17 ^a	1.94±0.28 ^a	2.08±0.20 ^a	
9	431-03-8	2,3-Butanedione	572.5	3.05	1.170	1.80±0.30 ^b	1.78±0.17 ^b	2.41±0.42 ^a	Butter, pastry, yeast
10	123-72-8	Butanal	574.2	3.07	1.115	0.67±0.13 ^b	0.55±0.08 ^a	0.70±0.12 ^a	Banana, green, pungent
		Butanal D	575	3.08	1.288	0.50±0.27 ^a	0.26±0.20 ^a	0.32±0.20 ^a	
11	78-85-3	2-Methyl-2-propenal	575.6	3.09	1.219	0.47±0.33 ^a	0.26±0.28 ^a	0.21±0.06 ^a	/
12	78-93-3	2-Butanone	582.7	3.16	1.251	3.61±0.68 ^a	2.76±0.61 ^b	2.51±0.96 ^b	Fragrant, fruit, pleasant
13	64-19-7	Acetic acid D	591.2	3.25	1.146	2.36±0.51 ^b	3.07±1.51 ^b	4.62±2.51 ^a	Acid, fruit, pungent, sour, vinegar
		Acetic acid	591.9	3.26	1.056	6.10±0.55 ^b	6.38±1.55 ^b	9.59±2.55 ^a	
14	141-78-6	Acetic acid ethyl ester D	596.7	3.32	1.338	1.14±1.93 ^b	1.51±2.93 ^a	0.51±3.93 ^{ab}	Aromatic, brandy, grape
		Acetic acid ethyl ester	599.2	3.34	1.097	0.96±0.56 ^b	1.53±0.13 ^a	1.45±0.27 ^a	

15	71-36-3	1-Butanol	641.7	3.86	1.164	1.98±0.22 ^a	1.68±0.46 ^a	2.01±0.21 ^a	Fruit
		1-Butanol D	641.8	3.87	1.398	3.71±0.59 ^a	2.68±0.95 ^b	2.25±1.08 ^b	
16	96-17-3	2-Methylbutanal D	653.6	4.02	1.400	3.60±0.61 ^a	3.03±0.83 ^{ab}	2.16±1.06 ^b	Almond, cocoa, fermented, hazelnut, malt
		2-Methylbutanal	654.6	4.04	1.159	1.92±0.23 ^a	1.71±0.44 ^a	1.96±0.15 ^a	
17	590-86-3	3-Methylbutanal	657.4	4.08	1.185	0.16±0.06 ^a	0.20±1.06 ^a	0.14±2.06 ^a	/
18	116-09-6	1-Hydroxy-2-propanone D	668.9	4.24	1.235	0.68±0.23 ^a	0.65±0.11 ^a	0.82±0.23 ^a	Butter, herb, malt, pungent
		1-Hydroxy-2-propanone	668.9	4.24	1.044	1.50±0.25 ^b	1.51±0.10 ^b	2.10±0.46 ^a	
19	29102	Propanoic acid	673.5	4.30	1.110	0.17±0.07 ^b	0.28±0.1 ^{ab}	0.36±0.16 ^a	Pungent
20	616-25-1	1-Penten-3-ol D	676.4	4.35	1.329	0.38±0.17 ^a	0.22±0.06 ^a	0.28±0.37 ^a	Butter, fish, green, oxidized, wet earth
		1-Penten-3-ol T	677.1	4.36	1.584	0.48±0.21 ^a	0.28±0.13 ^{ab}	0.26±0.16 ^b	
		1-Penten-3-ol	680.3	4.41	0.946	2.61±0.16 ^a	2.29±0.32 ^a	2.39±0.36 ^a	
21	1629-58-9	1-Penten-3-one D	683.5	4.45	1.313	0.85±0.64 ^a	0.34±0.31 ^{ab}	0.25±0.13 ^b	Fish, green, mustard, pungent
		1-Penten-3-one	683.8	4.46	1.078	1.10±0.52 ^a	0.54±0.44 ^b	0.59±0.18 ^b	
22	107-87-9	2-Pentanone	686.8	4.50	1.130	0.15±0.05 ^a	0.22±0.09 ^a	0.14±0.04 ^a	Fruit, pungent
23	96-22-0	3-Pentanone	689.6	4.56	1.103	0.35±0.15 ^a	0.21±1.15 ^a	0.32±2.15 ^a	/
24	600-14-6	2,3-Pentanedione	691.9	4.62	1.221	0.64±0.06 ^a	0.74±0.15 ^a	0.80±0.18 ^a	/
		2,3-Pentanedione D	691.9	4.63	1.306	0.13±0.06 ^a	0.09±0.05 ^a	0.14±0.05 ^a	
25	110-62-3	Pentanal D	693.3	4.67	1.423	1.99±0.91 ^a	1.07±0.69 ^b	1.32±1.69 ^{ab}	Almond, bitter, malt, oil, pungent
		Pentanal	694.3	4.69	1.182	1.62±0.43 ^a	1.09±0.39 ^b	1.66±0.29 ^a	
26	625-86-5	2,5-Dimethylfuran	693.4	4.67	1.343	0.18±0.04 ^a	0.17±0.08 ^a	0.22±0.05 ^a	Savory
27	3208-16-0	2-Ethylfuran	696.7	4.77	1.051	0.69±0.13 ^a	0.56±0.08 ^a	0.66±0.08 ^a	Butter, caramel
28	109-60-4	<i>n</i> -Propyl acetate	710.1	5.18	1.484	0.10±0.04 ^b	0.17±0.06 ^{ab}	0.47±0.46 ^a	Celery, floral, pear, red fruit
		<i>n</i> -Propyl acetate D	710.6	5.19	1.166	0.04±0.00 ^b	0.04±0.01 ^b	0.2±0.24 ^a	

29	513-86-0	3-Hydroxybutan-2-one	711.4	5.22	1.057	1.67±0.24 ^b	1.88±0.22 ^b	2.30±0.45 ^a	Butter, creamy, green pepper
30	763-32-6	3-Methyl-3-buten-1-ol	725.4	5.69	1.174	0.24±0.07 ^a	0.21±0.06 ^a	0.23±0.04 ^a	Cooked nut, fruit, herb, oil
31	108-10-1	Methyl isobutyl ketone	734.5	6.02	1.185	0.02±0.00 ^b	0.02±0.00 ^b	0.04±0.06 ^a	/
32	107-86-8	3-Methyl-2-butenal	745.1	6.43	1.087	0.31±0.18 ^a	0.38±0.14 ^a	0.43±0.07 ^a	Almond, roasted
33	1576-87-0	(<i>E</i>)-2-Pentenal D	748.8	6.58	1.364	0.23±0.19 ^a	0.08±0.11 ^b	0.06±0.03 ^b	/
		(<i>E</i>)-2-Pentenal	749.6	6.61	1.110	0.92±0.55 ^a	0.41±0.38 ^b	0.41±0.17 ^b	
34	71-41-0	Pentan-1-ol T	761.6	7.12	1.819	0.10±0.03 ^a	0.10±0.04 ^a	0.08±0.03 ^a	Balsamic, fruit, green, pungent, yeast
		Pentan-1-ol D	761.9	7.13	1.517	0.46±0.14 ^a	0.44±0.18 ^{ab}	0.29±0.16 ^b	
		Pentan-1-ol	762.9	7.18	1.257	1.60±0.28 ^a	1.58±0.39 ^a	1.33±0.42 ^a	
35	1576-95-0	(<i>Z</i>)-2-Penten-1-ol D	765.4	7.29	1.631	0.14±0.06 ^a	0.07±0.03 ^b	0.08±0.03 ^b	Banana, green, rubber
		(<i>Z</i>)-2-Penten-1-ol	766	7.31	0.942	2.27±0.36 ^a	1.66±0.40 ^b	1.79±0.34 ^b	
36	66-25-1	Hexanal D	797	8.70	1.563	1.90±1.05 ^a	0.85±0.67 ^b	0.78±0.36 ^b	Apple, fat, fresh, green, oil
		Hexanal	797.8	8.74	1.255	2.70±0.77 ^a	1.77±0.73 ^b	2.14±0.46 ^{ab}	
37	591-78-6	2-Hexanone	798	8.75	1.509	0.76±0.20 ^a	0.56±0.25 ^a	0.61±0.16 ^a	Fruity
38	141-79-7	Mesityl oxide	798.1	8.75	1.453	0.59±0.14 ^a	0.59±0.16 ^a	0.61±0.14 ^a	/
39	120-92-3	Cyclopentanone	799.3	8.80	1.106	0.98±0.29 ^b	1.16±0.35 ^{ab}	1.39±0.25 ^a	Mint, cool
40	693-95-8	4-Methylthiazole	818.3	9.63	1.051	1.47±0.00 ^a	2.19±0.00 ^a	2.01±0.00 ^a	Green, nut, roasted meat
41	123-86-4	Butyl acetate D	823.3	9.86	1.630	0.06±0.01 ^b	0.07±0.01 ^b	0.25±0.30 ^a	Apple, banana
		Butyl acetate	823.6	9.88	1.242	0.10±0.04 ^b	0.19±0.08 ^b	0.56±0.67 ^a	
42	105-30-6	2-Methyl-1-pentanol	838.7	10.62	1.286	0.05±0.03 ^a	0.10±0.07 ^a	0.04±0.01 ^a	/
43	623-36-9	2-Methyl-2-pentenal	845	10.94	1.163	0.11±0.03 ^a	0.09±0.06 ^a	0.08±0.04 ^a	Fruit
44	35796	Furfural	848.5	11.12	1.078	0.13±0.11 ^a	0.10±0.07 ^a	0.10±0.02 ^a	Almond, baked potatoes, bread, burnt, spice
45	2305-21-7	2-Hexen-1-ol D	865.5	12.06	1.515	0.11±0.06 ^a	0.05±0.05 ^b	0.04±0.02 ^b	Blue cheese, vegetable

		2-Hexen-1-ol	866	12.09	1.189	0.58±0.26 ^a	0.32±0.21 ^b	0.33±0.12 ^b	
46	928-96-1	(Z)-3-Hexen-1-ol	868.6	12.24	1.231	0.22±0.15 ^a	0.21±0.08 ^a	0.27±0.09 ^a	Grass, green fruit, green leaf, herb, unripe banana
		(Z)-3-Hexen-1-ol D	868.6	12.24	1.510	0.07±0.05 ^a	0.07±0.03 ^a	0.09±0.04 ^a	
47	111-27-3	<i>n</i> -Hexanol D	879.5	12.89	1.639	0.07±0.03 ^a	0.11±0.05 ^a	0.06±0.01 ^a	Banana, flower, grass, herb
		<i>n</i> -Hexanol	879.6	12.90	1.324	0.33±0.19 ^{ab}	0.52±0.25 ^a	0.28±0.08 ^b	
48	28588-74-1	2-Methyl-3-furanthiol	881.6	13.02	1.139	0.09±0.03 ^b	0.10±0.02 ^b	0.51±1.06 ^a	Fried, nut, potato, roasted meat
49	110-43-0	2-Heptanone	892.5	13.70	1.267	0.13±0.09 ^a	0.14±0.02 ^a	0.10±0.04 ^b	Blue cheese, fruit, green, nut, spice
50	6728-31-0	(Z)-4-Heptenal	901.5	13.96	1.158	0.31±0.18 ^a	0.19±0.14 ^a	0.18±0.04 ^a	Almond, fat, fruit
51	111-71-7	Heptanal D	903.2	14.01	1.699	0.69±0.36 ^a	0.39±0.16 ^b	0.62±0.13 ^a	Citrus, fat, green, nut
		Heptanal	904.2	14.04	1.325	1.23±0.33 ^a	0.90±0.25 ^b	1.33±0.21 ^a	Citrus, fat, green, nut
52	96-48-0	γ -Butyrolactone	927.7	14.73	1.083	0.15±0.03 ^b	0.21±0.09 ^{ab}	0.24±0.06 ^a	/
53	80-56-8	α -Pinene	932	14.86	1.222	0.10±0.10 ^b	0.25±0.13 ^a	0.04±0.01 ^b	Cedarwood, pine, sharp
54	1119-44-4	3-Hepten-2-one	938.4	15.06	1.218	0.11±0.12 ^b	0.30±0.17 ^a	0.04±0.07 ^b	Fruit
55	1003-04-9	4,5-Dihydro-3(2 <i>H</i>)-thiophenone	949.7	15.41	1.178	0.06±0.03 ^a	0.03±1.03 ^{ab}	0.02±2.03 ^b	Savory
56	100-52-7	Benzaldehyde	967.3	15.97	1.153	0.27±0.03 ^a	0.18±0.04 ^b	0.21±0.09 ^{ab}	Bitter almond, burnt sugar, cherry, malt, roasted pepper
		Benzaldehyde D	967.2	15.97	1.477	0.04±0.01 ^a	0.03±0.01 ^b	0.03±0.02 ^b	
57	127-91-3	β -Pinene	977.2	16.30	1.214	0.40±0.44 ^{ab}	1.10±0.30 ^a	0.10±0.07 ^b	Pine, polish, wood
		β -Pinene D	977.2	16.30	1.639	0.02±0.02 ^b	0.07±0.03 ^a	0.02±0.00 ^b	
		β -Pinene T	977.9	16.33	1.733	0.02±0.01 ^b	0.05±0.02 ^a	0.02±0.00 ^b	
58	589-98-0	3-Octanol	988.2	16.67	1.391	0.19±0.04 ^{ab}	0.16±1.04 ^b	0.21±2.04 ^a	Citrus, moss, mushroom, nut, oil
59	13360-64-0	2-Ethyl-5-methylpyrazine	992.1	16.81	1.181	0.21±0.043 ^a	0.20±0.03 ^a	0.19±0.07 ^a	Fruit, green
60	123-35-3	Myrcene D	993.1	16.84	1.286	0.07±0.03 ^a	0.14±0.14 ^a	0.03±0.00 ^b	Balsamic, fruit, geranium, herb, must
		Myrcene T	993	16.84	1.716	0.05±0.02 ^a	0.12±0.13 ^a	0.05±0.01 ^a	

		Myrcene	993.7	16.86	1.222	0.20±0.09 ^a	0.39±0.34 ^a	0.08±0.01 ^b	
61	3777-69-3	2-Pentylfuran	994.2	16.88	1.258	0.24±0.07 ^a	0.18±0.05 ^a	0.16±0.07 ^a	Butter, floral, fruit, green bean
62	13925-03-6	2-Ethyl-6-methylpyrazine	1001	17.11	1.195	0.09±0.07 ^a	0.04±0.04 ^b	0.03±0.01 ^b	Green, nuts, roasted
63	124-13-0	Octanal D	1005.4	17.25	1.824	0.03±0.02 ^a	0.02±0.00 ^b	0.03±0.00 ^a	Citrus, fat, green, oil, pungent
		Octanal	1005.5	17.26	1.408	0.17±0.07 ^a	0.10±0.02 ^b	0.15±0.02 ^{ab}	
64	5910-85-0	2,4-Heptadienal	1014.2	17.55	1.623	0.43±0.30 ^a	0.18±0.18 ^b	0.15±0.08 ^b	Fat, nut
		2,4-Heptadienal D	1015.1	17.58	1.195	0.12±0.10 ^a	0.05±0.05 ^b	0.04±0.01 ^b	
65	13466-78-9	3-Carene D	1030.2	18.11	1.727	0.09±0.03 ^b	0.19±0.16 ^a	0.09±0.02 ^b	Lemon
		3-Carene	1030.1	18.11	1.666	0.06±0.02 ^b	0.15±0.13 ^a	0.05±0.01 ^b	
66	138-86-3	Limonene	1030.5	18.12	1.225	0.40±0.20 ^a	0.85±0.50 ^a	0.08±0.02 ^b	Citrus, mint
		Limonene D	1030.4	18.12	1.290	0.44±0.23 ^a	0.89±0.50 ^a	0.09±0.02 ^b	
67	470-82-6	1,8-Cineole D	1034.4	18.26	1.727	0.06±0.03 ^b	0.20±0.17 ^a	0.04±0.01 ^b	Camphor, cool, eucalyptol, mint
		1,8-Cineole	1034.8	18.27	1.290	0.40±0.25 ^b	0.98±0.52 ^a	0.10±0.03 ^a	
68	100-51-6	Benzenemethanol	1054.2	18.98	1.173	0.08±0.03 ^b	0.14±0.05 ^a	0.14±0.04 ^a	Boiled cherries, moss, roasted bread, rose
69	15707-34-3	2,3-Dimethyl-5-ethylpyrazine D	1074	19.73	1.745	0.13±0.07 ^a	0.07±0.04 ^b	0.07±0.03 ^{ab}	Burnt, green bean, popcorn
		2,3-Dimethyl-5-ethylpyrazine	1074.4	19.74	1.215	0.35±0.15 ^a	0.24±0.12 ^{ab}	0.19±0.11 ^b	
70	626-77-7	Propyl hexanoate	1079.2	19.92	1.391	0.05±0.02 ^a	0.08±0.06 ^a	0.06±0.02 ^a	Berry, fruit, petrol, pineapple, roasted garlic
71	78-70-6	Linalool	1104.9	20.95	1.225	0.29±0.08 ^b	0.54±0.25 ^a	0.33±0.12 ^b	Coriander, floral, lavender, lemon, rose
72	124-19-6	Nonanal D	1107.9	21.07	1.954	0.11±0.06 ^a	0.06±0.01 ^b	0.10±0.01 ^{ab}	Fat, floral, green, lemon
		Nonanal	1108.4	21.09	1.466	0.45±0.16 ^a	0.28±0.05 ^b	0.42±0.05 ^a	
73		Unknown compound 1	552.2	2.85	1.161	0.60±0.11 ^b	0.62±0.11 ^b	0.88±0.21 ^a	/
74		Unknown compound 2	550.6	2.83	1.190	0.51±0.09 ^a	0.64±0.19 ^a	0.51±0.10 ^a	/
75		Unknown compound 3	565.9	2.99	1.030	0.79±0.31 ^a	1.12±0.38 ^a	1.13±0.49 ^a	/

76		Unknown compound 4	583.5	3.17	1.192	0.87±0.38 ^a	0.63±0.31 ^a	0.91±0.15 ^a	/
77		Unknown compound 5	597.8	3.33	1.235	0.27±0.23 ^b	0.76±0.53 ^a	0.41±0.14 ^b	/
78		Unknown compound 6	550.1	2.83	1.283	0.85±0.18 ^a	0.73±0.17 ^a	0.56±0.42 ^a	/
79		Unknown compound 7	677.9	4.37	1.279	0.31±0.09 ^a	0.22±0.06 ^b	0.17±0.01 ^b	/
80		Unknown compound 8	736	6.08	1.078	0.29±0.09 ^b	0.25±0.03 ^b	0.37±0.07 ^a	/
81		Unknown compound 9	757.1	6.92	1.124	0.10±0.11 ^a	0.04±0.01 ^a	0.04±0.00 ^a	/
82		Unknown compound 10	737.3	6.12	1.099	0.14±0.04 ^a	0.12±0.06 ^a	0.12±0.05 ^a	/
83		Unknown compound 11	932.5	14.88	1.284	0.10±0.06 ^a	0.20±0.10 ^a	0.08±0.30 ^a	/
84		Unknown compound 12	587.8	3.22	1.091	0.52±0.13 ^b	0.64±0.15 ^b	0.93±0.22 ^a	/

3 Different superscript letters (a, b) in the same row indicate significant differences ($p < 0.05$). D and T in the compound names indicate IMS-formed adducts, dimers and trimers,
4 respectively. RI, retention index, Rt, retention time (min); Dt, drift time (ms). The aroma characteristics are based on information from <https://www.femaflavor.org> (June 30, 2025).

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