Supplementary information

Geographical origin traceability analysis of Camellia oil based on headspace gas chromatography–ion mobility spectrometry and chemometrics

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Tabel S1 The information of VOCs in samples identified by GC–IMS.

No.	Compound	Formula	RI	Rt [sec]	Dt [a.u.]	Comment
Aldehydes						
1	n-Nonanal	$C_9H_{18}O$	1111.1	569.688	147.103	Monomer
2	n-Nonanal	$C_9H_{18}O$	1111.7	570.783	194.096	Dimer
3	2-phenylacetaldehyde	C_8H_8O	1049.1	457.91	125.222	Monomer
4	2-phenylacetaldehyde	C_8H_8O	1045.8	452.592	153.422	Dimer
5	n-Octanal	$C_8H_{16}O$	1010.0	399.027	140.091	Dimer
6	n-Octanal	$C_8H_{16}O$	1010.6	399.815	181.988	Monomer
7	(E)-2-Heptenal	$C_7H_{12}O$	962.4	343.777	125.662	Monomer
8	(E)-2-Heptenal	$C_7H_{12}O$	962.4	343.777	167.003	Dimer
9	Heptanal	$C_7H_{14}O$	907.2	291.638	13.312	Monomer
10	Heptanal	$C_7H_{14}O$	907.0	291.436	169.745	Dimer
11	(Z)-4-heptenal	$C_7H_{12}O$	902.5	287.643	16.118	
12	2-Hexenal	$C_6H_{10}O$	853.7	253.619	117.938	Monomer
13	2-Hexenal	$C_6H_{10}O$	852.9	253.104	151.795	Dimer
14	2-furfural	$C_5H_4O_2$	835.7	242.562	108.435	Monomer
15	2-furfural	$C_5H_4O_2$	834.0	241.533	132.986	Dimer
16	1-hexanal	$C_6H_{12}O$	794.3	219.009	126.141	Monomer
17	1-hexanal	$C_6H_{12}O$	796.4	220.143	156.468	Dimer
18	Pentanal	$C_5H_{10}O$	727.5	186.186	118.075	Monomer
19	Pentanal	$C_5H_{10}O$	728.0	186.396	141.909	Dimer
20	n-pentanal	$C_5H_{10}O$	703.0	175.476	118.711	Monomer
21	n-pentanal	$C_5H_{10}O$	702.6	175.266	142.703	Dimer
22	Butanal	C_4H_8O	609.1	146.406	129.029	
23	Butanal	C_4H_8O	576.6	137.92	128.379	
24	3-Methyl-2-butenal	C5H8O	783.1	213.043	135.964	
25	(E)-2-Octenal	$C_8H_{14}O$	1063.3	481.434	133.488	
26	2-Methyl-2-propenal	C_4H_6O	569.7	136.158	122.287	
Ketones						
27	Cyclohexanone	$C_6H_{10}O$	897.2	283.095	115.238	Monomer
28	Cyclohexanone	$C_6H_{10}O$	897.0	282.94	145.265	Dimer
29	2-Heptanone	$C_7H_{14}O$	895.8	281.912	125.992	Monomer
30	2-Heptanone	$C_7H_{14}O$	895.6	281.722	163.174	Dimer
31	Acetoin	$C_4H_8O_2$	719.0	182.406	105.682	Monomer
32	Acetoin	$C_4H_8O_2$	718.8	182.301	13.317	Dimer
33	2-Pentanone	$C_5H_{10}O$	690.7	170.317	137.444	
34	2-Octanone	$C_8H_{16}O$	998.8	383.56	13.334	Monomer
35	2-Octanone	$C_8H_{16}O$	998.0	382.496	175.542	Dimer
36	2-Hexanone	$C_6H_{12}O$	786.4	214.759	119.014	Monomer
37	2-Hexanone	$C_6H_{12}O$	786.4	214.759	150.885	Dimer
38	2,3-Butanedione	$C_4H_6O_2$	590.8	141.548	118.516	
39	2-Butanone	C_4H_8O	596.3	142.998	124.911	
40	2-Propanone	C_3H_6O	499.4	119.669	1.12	
Alcohols						
41	1-Heptanol	$C_7H_{16}O$	980.6	362.886	14.013	Monomer
42	1-Heptanol	$C_7H_{16}O$	979.8	361.98	176.389	Dimer
43	1-Hexanol	$C_6H_{14}O$	874.6	267.072	132.453	Monomer
44	1-Hexanol	$C_6H_{14}O$	874.1	266.712	163.561	Dimer
45	1-Pentanol	$C_5H_{12}O$	765.5	204.143	125.486	Monomer
46	1-Pentanol	$C_5H_{12}O$	766.4	204.592	151.329	Dimer
47	3-methylbutanol	$C_5H_{12}O$	738.8	191.337	148.688	
48	1-Propanol, 2-methyl	$C_4H_{10}O$	630.6	152.297	116.995	Monomer
49	1-Propanol, 2-methyl	$C_4H_{10}O$	629.6	152.043	136.396	Dimer

50	2.3-Butanediol	$C_4H_{10}O_2$	791.2	217.286	136.151	
51	1-Octanol	$C_8H_{18}O$	1080.3	511.084	146.825	
52	Ethanol	C_2H_6O	455.8	110.437	105.375	Monomer
53	Ethanol	C_2H_6O	455.8	110.437	113.356	Dimer
Esters						
54	Dihydro-5-methyl-2(3H)-furanone	$C_5H_8O_2$	959.3	340.566	113.323	Monomer
56	Dihydro-5-methyl-2(3H)-furanone	$C_5H_8O_2$	960.0	341.286	14.168	Dimer
57	γ-Butyrolactone	$C_4H_6O_2$	919.4	302.423	108.247	Monomer
58	γ-Butyrolactone	$C_4H_6O_2$	918.4	301.552	129.848	Dimer
59	2-Methylbutanol acetate	$C_7H_{14}O_2$	882.8	272.493	129.805	Monomer
60	2-Methylbutanol acetate	$C_7H_{14}O_2$	881.9	271.922	173.852	Dimer
61	Ethyl 2-methylbutanoate	$C_7H_{14}O_2$	849.6	251.047	124.076	Monomer
62	Ethyl 2-methylbutanoate	$C_7H_{14}O_2$	850.4	251.562	165.061	Dimer
63	ethyl 2-methylpropanoate	$C_6H_{12}O_2$	756.7	199.809	119.413	Monomer
64	ethyl 2-methylpropanoate	$C_6H_{12}O_2$	755.5	199.238	156.175	Dimer
65	Ethyl acetate	$C_4H_8O_2$	622.8	150.154	133.751	
66	3-Methylbutyl acetate	$C_7H_{14}O_2$	860.0	257.591	130.939	
67	methyl acetate	$C_3H_6O_2$	551.3	131.639	119.767	
68	ethyl 2-hydroxypropanoate	$C_5H_{10}O_3$	813.4	229.593	113.986	
Acids						
69	Hexanoic acid	$C_6H_{12}O_2$	999.8	384.879	129.769	
70	2-Methylpropanoic acid	$C_4H_8O_2$	758.2	200.557	138.247	
71	2-methylbutanoic acid	$C_5H_{10}O_2$	851.2	252.029	120.018	Monomer
72	2-methylbutanoic acid	$C_5H_{10}O_2$	851.4	252.175	147.192	Dimer
73	Propanoic acid	$C_3H_6O_2$	682.7	167.609	110.781	
74	3-methylbutanoic acid	$C_5H_{10}O_2$	839.9	245.112	122.011	
75	Acetic acid	$C_2H_4O_2$	596.7	143.091	115.074	
Other						
76	Camphene	$C_{10}H_{16}$	943.8	325.206	11.952	Monomer
77	Camphene	$C_{10}H_{16}$	944.3	325.686	164.214	Dimer
78	1-Octene	C_8H_{16}	786.9	215.021	144.592	
79	2-phenyl-1,3-dioxolane-4-methanol	$C_{10}H_{12}O_3$	967.5	349.036	115.287	Monomer
80	2-phenyl-1,3-dioxolane-4-methanol	$C_{10}H_{12}O_3$	966.8	348.227	146.732	Dimer
81	2-Pentylfuran	$C_9H_{14}O$	999.4	384.3	12.552	
82	2,5-Dimethylpyrazine	$C_6H_8N_2$	914.5	298.074	111.339	
83	2,3,5-trimethylpyrazine	$C_7H_{10}N_2$	1010.3	399.411	11.746	
84	Dimethyl disulfide	$C_2H_6S_2$	720.3	182.955	114.311	
85	3-Butenenitrile	C_4H_5N	638.3	154.479	125.461	

Table S2 Confusion matrix of discriminant analysis results at province-level.

Algorithm	True Class	Predicted ZJ	Predicted YN	Predicted HB	Predicted HN	Predicted CQ	Predicted JX	Predicted GZ
PLS-DA	ZJ	6	0	0	0	0	0	0
	YN	0	6	0	0	0	0	0
	HB	0	0	6	0	0	0	0
	HN	0	0	0	18	0	0	0
	CQ	0	0	0	0	6	0	0
	JX	0	0	0	1	0	17	0
	GZ	0	0	0	1	0	0	5
	Total	6	6	6	20	6	17	5
SPA-PLS-DA	ZJ	6	0	0	0	0	0	0
	YN	0	6	0	0	0	0	0
	HB	0	0	6	0	0	0	0
	HN	0	0	0	18	0	0	0
	CQ	0	0	0	0	6	0	0
	JX	0	0	0	0	0	18	0
	GZ	0	0	0	0	0	0	6
	Total	6	6	6	18	6	18	6

Table S3 Confusion matrix of discriminant analysis results at city-level.

Algorithm	True Class	Predicted ZJ-CS	Predicted JX-GZ	Predicted GZ-LP	Predicted YN-TC	Predicted HB-HS	Predicted HN-SY	Predicted HN-LY	Predicted HN-HY	Predicted CQ-YY	Predicted JX-GX	Predicted JX-YS
PLS-DA	ZJ-CS	6	0	0	0	0	0	0	0	0	0	0
	JX-GZ	0	6	0	0	0	0	0	0	0	0	0
	GZ-LP	0	0	6	0	0	0	0	0	0	0	0
	YN-TC	0	0	0	6	0	0	0	0	0	0	0
	HB-HS	0	0	0	0	6	0	0	0	0	0	0
	HN-SY	0	0	0	0	0	6	0	0	0	0	0
	HN-LY	0	0	0	0	0	0	6	0	0	0	0
	HN-HY	0	0	0	0	0	0	0	6	0	0	0
	CQ-YY	0	0	0	0	0	0	0	0	6	0	0
	JX-GX	0	0	0	0	0	0	0	0	0	6	0
	JX-YS	0	0	0	0	0	0	0	0	0	0	6
	Total	6	6	6	6	6	6	6	6	6	6	6
SPA-PLS-DA	ZJ-CS	6	0	0	0	0	0	0	0	0	0	0
	JX-GZ	0	6	0	0	0	0	0	0	0	0	0
	GZ-LP	0	0	6	0	0	0	0	0	0	0	0
	YN-TC	0	0	0	6	0	0	0	0	0	0	0
	HB-HS	0	0	0	0	6	0	0	0	0	0	0
	HN-SY	0	0	0	0	0	6	0	0	0	0	0
	HN-LY	0	0	0	0	0	0	6	0	0	0	0
	HN-HY	0	0	0	0	0	0	0	6	0	0	0
	CQ-YY	0	0	0	0	0	0	0	0	6	0	0
	JX-GX	0	0	0	0	0	0	0	0	1	5	0
	JX-YS	0	0	0	0	0	0	0	0	0	0	6
	Total	6	6	6	6	6	6	6	6	7	5	6