

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

Shaojie Wu^a, Haojie Wu^{a,b}, Jirong Wu^b, You Zhou^{b,c}, Tingting Han^b, Daoming Chen^b,
Jianbo Qiu^{b,c}, Xin Liu^{b,c}, Jianrong Shi^{b,c}, Jianhong Xu^{b,c}, Guanghui Shen^{a,b,c,*}

^a School of Ocean Food and Biological Engineering, Jiangsu Ocean University, Lianyungang, Jiangsu, China

^b Jiangsu Key Laboratory for Food Quality and Safety-State Key Laboratory Cultivation Base, Ministry of Science and Technology/Key Laboratory for Agro-product Safety Risk Evaluation (Nanjing), Ministry of Agriculture and Rural Affairs/Collaborative Innovation Center for Modern Grain Circulation and Safety/Institute of Food Safety and Nutrition, Jiangsu Academy of Agricultural Sciences, Nanjing, China

^c School of Food and Biological Engineering, Jiangsu University, Zhenjiang, Jiangsu, China

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 ₉ H ₁₈ O	1111.1	569.688	147.103	Monomer
2	n-Nonanal	C ₉ H ₁₈ O	1111.7	570.783	194.096	Dimer
3	2-phenylacetaldehyde	C ₈ H ₈ O	1049.1	457.91	125.222	Monomer
4	2-phenylacetaldehyde	C ₈ H ₈ O	1045.8	452.592	153.422	Dimer
5	n-Octanal	C ₈ H ₁₆ O	1010.0	399.027	140.091	Dimer
6	n-Octanal	C ₈ H ₁₆ O	1010.6	399.815	181.988	Monomer
7	(E)-2-Heptenal	C ₇ H ₁₂ O	962.4	343.777	125.662	Monomer
8	(E)-2-Heptenal	C ₇ H ₁₂ O	962.4	343.777	167.003	Dimer
9	Heptanal	C ₇ H ₁₄ O	907.2	291.638	13.312	Monomer
10	Heptanal	C ₇ H ₁₄ O	907.0	291.436	169.745	Dimer
11	(Z)-4-heptenal	C ₇ H ₁₂ O	902.5	287.643	16.118	
12	2-Hexenal	C ₆ H ₁₀ O	853.7	253.619	117.938	Monomer
13	2-Hexenal	C ₆ H ₁₀ O	852.9	253.104	151.795	Dimer
14	2-furfural	C ₅ H ₄ O ₂	835.7	242.562	108.435	Monomer
15	2-furfural	C ₅ H ₄ O ₂	834.0	241.533	132.986	Dimer
16	1-hexanal	C ₆ H ₁₂ O	794.3	219.009	126.141	Monomer
17	1-hexanal	C ₆ H ₁₂ O	796.4	220.143	156.468	Dimer
18	Pentanal	C ₅ H ₁₀ O	727.5	186.186	118.075	Monomer
19	Pentanal	C ₅ H ₁₀ O	728.0	186.396	141.909	Dimer
20	n-pentanal	C ₅ H ₁₀ O	703.0	175.476	118.711	Monomer
21	n-pentanal	C ₅ H ₁₀ O	702.6	175.266	142.703	Dimer
22	Butanal	C ₄ H ₈ O	609.1	146.406	129.029	
23	Butanal	C ₄ H ₈ O	576.6	137.92	128.379	
24	3-Methyl-2-butenal	C ₅ H ₈ O	783.1	213.043	135.964	
25	(E)-2-Octenal	C ₈ H ₁₄ O	1063.3	481.434	133.488	
26	2-Methyl-2-propenal	C ₄ H ₆ O	569.7	136.158	122.287	
Ketones						
27	Cyclohexanone	C ₆ H ₁₀ O	897.2	283.095	115.238	Monomer
28	Cyclohexanone	C ₆ H ₁₀ O	897.0	282.94	145.265	Dimer
29	2-Heptanone	C ₇ H ₁₄ O	895.8	281.912	125.992	Monomer
30	2-Heptanone	C ₇ H ₁₄ O	895.6	281.722	163.174	Dimer
31	Acetoin	C ₄ H ₈ O ₂	719.0	182.406	105.682	Monomer
32	Acetoin	C ₄ H ₈ O ₂	718.8	182.301	13.317	Dimer
33	2-Pentanone	C ₅ H ₁₀ O	690.7	170.317	137.444	
34	2-Octanone	C ₈ H ₁₆ O	998.8	383.56	13.334	Monomer
35	2-Octanone	C ₈ H ₁₆ O	998.0	382.496	175.542	Dimer
36	2-Hexanone	C ₆ H ₁₂ O	786.4	214.759	119.014	Monomer
37	2-Hexanone	C ₆ H ₁₂ O	786.4	214.759	150.885	Dimer
38	2,3-Butanedione	C ₄ H ₆ O ₂	590.8	141.548	118.516	
39	2-Butanone	C ₄ H ₈ O	596.3	142.998	124.911	
40	2-Propanone	C ₃ H ₆ O	499.4	119.669	1.12	
Alcohols						
41	1-Heptanol	C ₇ H ₁₆ O	980.6	362.886	14.013	Monomer
42	1-Heptanol	C ₇ H ₁₆ O	979.8	361.98	176.389	Dimer
43	1-Hexanol	C ₆ H ₁₄ O	874.6	267.072	132.453	Monomer
44	1-Hexanol	C ₆ H ₁₄ O	874.1	266.712	163.561	Dimer
45	1-Pentanol	C ₅ H ₁₂ O	765.5	204.143	125.486	Monomer
46	1-Pentanol	C ₅ H ₁₂ O	766.4	204.592	151.329	Dimer
47	3-methylbutanol	C ₅ H ₁₂ O	738.8	191.337	148.688	
48	1-Propanol, 2-methyl	C ₄ H ₁₀ O	630.6	152.297	116.995	Monomer
49	1-Propanol, 2-methyl	C ₄ H ₁₀ O	629.6	152.043	136.396	Dimer

50	2,3-Butanediol	C ₄ H ₁₀ O ₂	791.2	217.286	136.151	
51	1-Octanol	C ₈ H ₁₈ O	1080.3	511.084	146.825	
52	Ethanol	C ₂ H ₆ O	455.8	110.437	105.375	Monomer
53	Ethanol	C ₂ H ₆ O	455.8	110.437	113.356	Dimer
Esters						
54	Dihydro-5-methyl-2(3H)-furanone	C ₅ H ₈ O ₂	959.3	340.566	113.323	Monomer
56	Dihydro-5-methyl-2(3H)-furanone	C ₅ H ₈ O ₂	960.0	341.286	14.168	Dimer
57	γ-Butyrolactone	C ₄ H ₆ O ₂	919.4	302.423	108.247	Monomer
58	γ-Butyrolactone	C ₄ H ₆ O ₂	918.4	301.552	129.848	Dimer
59	2-Methylbutanol acetate	C ₇ H ₁₄ O ₂	882.8	272.493	129.805	Monomer
60	2-Methylbutanol acetate	C ₇ H ₁₄ O ₂	881.9	271.922	173.852	Dimer
61	Ethyl 2-methylbutanoate	C ₇ H ₁₄ O ₂	849.6	251.047	124.076	Monomer
62	Ethyl 2-methylbutanoate	C ₇ H ₁₄ O ₂	850.4	251.562	165.061	Dimer
63	ethyl 2-methylpropanoate	C ₆ H ₁₂ O ₂	756.7	199.809	119.413	Monomer
64	ethyl 2-methylpropanoate	C ₆ H ₁₂ O ₂	755.5	199.238	156.175	Dimer
65	Ethyl acetate	C ₄ H ₈ O ₂	622.8	150.154	133.751	
66	3-Methylbutyl acetate	C ₇ H ₁₄ O ₂	860.0	257.591	130.939	
67	methyl acetate	C ₃ H ₆ O ₂	551.3	131.639	119.767	
68	ethyl 2-hydroxypropanoate	C ₅ H ₁₀ O ₃	813.4	229.593	113.986	
Acids						
69	Hexanoic acid	C ₆ H ₁₂ O ₂	999.8	384.879	129.769	
70	2-Methylpropanoic acid	C ₄ H ₈ O ₂	758.2	200.557	138.247	
71	2-methylbutanoic acid	C ₅ H ₁₀ O ₂	851.2	252.029	120.018	Monomer
72	2-methylbutanoic acid	C ₅ H ₁₀ O ₂	851.4	252.175	147.192	Dimer
73	Propanoic acid	C ₃ H ₆ O ₂	682.7	167.609	110.781	
74	3-methylbutanoic acid	C ₅ H ₁₀ O ₂	839.9	245.112	122.011	
75	Acetic acid	C ₂ H ₄ O 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 ₈ H 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 ₉ H ₁₄ O	999.4	384.3	12.552	
82	2,5-Dimethylpyrazine	C ₆ H ₈ N ₂	914.5	298.074	111.339	
83	2,3,5-trimethylpyrazine	C ₇ H ₁₀ N ₂	1010.3	399.411	11.746	
84	Dimethyl disulfide	C ₂ H ₆ S ₂	720.3	182.955	114.311	
85	3-Butenenitrile	C ₄ H ₅ N	638.3	154.479	125.461	

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

Algorithm	True	Predicted	Predicted	Predicted	Predicted	Predicted	Predicted	Predicted
	Class	ZJ	YN	HB	HN	CQ	JX	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.

[illegible]