

附表 1 盐源与汉源花椒籽挥发油成分及相对含量

Supplementary 1 The volatile oil components and relative content of *Zanthoxylum bungeanum* seeds from Yanyuan and Hanyuan

序号 NO.	化合物名称 Compound name	分子式 Formula	保留时间 Retention time(min)	各花椒籽样品挥发油成分相对含量百分比 Relative percentage content of volatile oil components in various <i>Zanthoxylum bungeanum</i> seeds samples (%)														分类 Classification
				盐源 Yanyuan							汉源 Hanyuan							
				1	2	3	4	5	6	1	2	3	4	5	6	7		
1	(Z)-3-辛烯-2-醇 (Z)-3-Octen-2-ol	C ₈ H ₁₆ O	4.324	0.15	0.09	0.08	0.05	0.08	0.08	0.10	0.05	0.08	-	0.06	0.21	-	醇类 Alcohols	
2	(E)-2-己烯醛 (E)-2-Hexenal	C ₆ H ₁₀ O	5.013	0.05	0.03	-	-	-	-	0.06	-	0.04	-	0.07	-	0.02	醛类 Aldehydes	
3	正己醇 1-Hexanol	C ₆ H ₁₄ O	5.433	-	0.12	-	-	-	0.11	0.58	0.22	0.40	0.27	0.66	0.44	0.28	醇类 Alcohols	
4	2-庚酮 2-Heptanone	C ₇ H ₁₄ O	6.040	0.14	0.15	0.09	-	0.10	0.10	0.47	0.10	0.13	0.14	0.42	0.24	0.11	酮类 Ketones	
5	2-正丁基呋喃 2-n-Butyl furan	C ₈ H ₁₂ O	6.059	-	0.21	-	-	-	0.14	-	-	0.25	0.16	0.41	0.38	0.13	呋喃类 Furan derivatives	
6	庚醛 Heptanal	C ₇ H ₁₄ O	6.433	-	1.17	1.02	-	1.10	0.82	2.96	1.12	1.53	1.42	3.91	3.24	1.31	醛类 Aldehydes	
7	2-乙基苯酚 2-ethyl-Phenol	C ₈ H ₁₀ O	6.999	0.03	0.04	-	-	-	-	-	-	-	-	0.04	-	-	酚类 Phenols	
8	α -侧柏烯 α -thuiene	C ₁₀ H ₁₆	7.319	0.07	0.06	0.04	-	0.04	0.06	-	-	-	0.02	-	-	-	萜烯类 Terpenes	

21	3-(2-甲基丙基)-1-环己烯 3-(2-methylpropyl)-Cyclohexane	C ₁₈ H ₁₀	10.270	3.03	4.90	3.30	2.97	3.83	4.52	4.45	3.04	3.96	3.37	4.74	4.44	2.77	烯烃类 Olefins
22	正辛醛 Octanal	C ₈ H ₁₆ O	11.033	1.27	1.15	0.83	0.39	0.86	0.88	2.95	1.39	2.13	1.65	3.70	2.94	1.87	醛类 Aldehydes
23	反式-2,4-庚二烯醛 trans-2,4-Heptadienal	C ₇ H ₁₀ O	11.426	-	-	-	-	-	-	0.05	-	-	-	0.11	-	-	醛类 Aldehydes
24	松油烯 1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)	C ₁₀ H ₁₆	11.724	0.06	0.05	-	-	-	-	-	-	-	0.03	-	-	-	萜烯类 Terpenes
25	D-柠檬烯 D-Limonene*	C ₁₀ H ₁₆	12.524	20.47	25.81	17.72	16.36	20.43	21.92	22.30	13.10	14.27	13.86	19.78	16.12	12.19	萜烯类 Terpenes
26	桉叶油醇 Cineole	C ₁₀ H ₁₈ O	12.677	6.47	6.25	4.31	2.23	4.92	5.28	4.26	2.67	3.58	3.66	4.58	3.43	3.73	环醚类 Cyclic ethers
27	反式-β-罗勒烯 trans-β-Ocimene	C ₁₀ H ₁₆	13.099	0.18	0.54	0.26	0.61	0.53	0.59	0.69	0.30	0.24	0.21	0.38	0.14	0.22	萜烯类 Terpenes
28	反式-3-辛烯-2-酮 trans-3-Octen-2-one	C ₈ H ₁₄ O	13.175	0.15	0.18	0.10	-	-	-	-	-	-	0.11	0.28	0.14	0.14	酮类 Ketones
29	β-罗勒烯 β-Ocimene	C ₁₀ H ₁₆	13.788	0.33	0.67	0.31	0.65	0.47	0.58	1.01	0.49	0.32	0.32	0.51	0.21	0.33	萜烯类 Terpenes
30	反式-2-辛烯醛 trans-2-Octenal	C ₈ H ₁₄ O	14.569	0.42	0.61	0.33	0.15	0.34	0.34	1.53	0.79	1.09	1.03	1.64	1.33	1.30	醛类 Aldehydes
31	环氧芳樟醇 Linalool Oxide	C ₁₀ H ₁₈ O ₂	15.439	1.00	1.16	0.71	0.34	0.78	0.52	1.15	0.84	0.53	1.50	1.11	0.39	0.82	醇类 Alcohols
32	辛醇 Octanol	C ₈ H ₁₈ O	15.679	0.24	0.38	0.23	0.21	0.23	0.22	1.65	0.73	1.16	0.84	1.91	1.43	1.06	醇类 Alcohols

33	3-萜烯 3-Carene	C ₁₀ H ₁₆	16.389	0.16	0.12	-	-	-	0.08	-	-	-	-	-	-	-	萜烯类 Terpenes
34	反式芳樟醇氧化物 trans-Linalool oxide	C ₁₀ H ₁₈ O ₂	16.582	0.61	0.79	0.48	0.19	0.52	0.30	1.03	0.53	0.37	1.08	0.87	0.29	0.63	醇类 Alcohols
35	2-壬酮 2-Nonanone	C ₉ H ₁₈ O	16.976	-	-	-	-	-	-	-	-	-	-	0.32	0.22	-	酮类 Ketones
36	芳樟醇 Linalool*	C ₁₀ H ₁₈ O	17.680	13.51	11.94	5.65	6.83	8.94	9.98	3.91	4.17	2.63	4.67	4.23	2.56	3.62	醇类 Alcohols
37	壬醛 Nonanal*	C ₉ H ₁₈ O	17.961	1.1	1.09	0.84	0.72	0.79	0.84	2.61	1.31	2.23	1.56	3.29	2.93	2.14	醛类 Aldehydes
38	6-异丙烯基-3-甲氧基甲氧基 -3-甲基-环己烯 6-Isopropenyl-3-methoxymethoxy-3-methyl-cyclohexene	C ₁₂ H ₂₀ O ₂	18.185	-	-	-	-	-	-	-	0.11	-	0.14	-	-	-	烯烃类 Olefins
39	反式-1-甲基-4-(1-甲基乙基)环己-2-烯-1-醇 trans-2-Cyclohexen-1-ol,1-methyl-4-(1-methylethenyl)	C ₁₀ H ₁₆ O	18.865	0.52	0.70	0.35	0.19	0.40	0.30	0.31	0.31	0.24	0.57	0.44	0.18	0.46	醇类 Alcohols
40	α -龙脑烯醛 α -Campholenal	C ₁₀ H ₁₆ O	19.109	-	-	-	-	-	-	-	-	-	0.07	-	-	0.12	醛类 Aldehydes
41	柠檬烯环氧化物 Limonene oxide	C ₁₀ H ₁₆ O	19.532	0.32	0.33	0.22	0.17	0.26	0.23	0.60	0.31	0.26	0.53	0.57	0.47	0.35	萜烯类 Terpenes
42	反式-柠檬烯环氧化物 trans-Limonene oxide	C ₁₀ H ₁₆ O	19.787	-	-	-	-	-	-	1.49	0.87	0.88	-	1.43	1.17	1.30	萜烯类 Terpenes

	1-异丙烯基-4-甲基-1,2-环己 二醇																	
43	(1S-(1Alpha,2alpha,4beta)-1-isopropenyl-4-methyl-1,2-cyclohexanediol	C ₁₀ H ₁₈ O ₂	19.814	1.5	1.37	0.91	0.42	0.74	0.62	-	-	-	1.36	-	-	-	-	醇类 Alcohols
44	3-壬烯-2-酮 3-Nonen-2-one	C ₉ H ₁₆ O	20.068	-	0.08	-	-	-	-	-	-	-	-	0.24	-	-	-	酮类 Ketones
45	2,2-二甲基-3-[(2Z)-3-甲基戊-2,4-二烯基]环氧乙烷 (Z)-2,2-Dimethyl-3-(3-methylpenta-2,4-dien-1-yl)oxirane	C ₁₀ H ₁₆ O	20.111	-	-	-	-	-	-	0.22	0.21	-	0.33	-	-	0.27	-	萜类环氧化物 Terpenoid epoxides
46	反式-马鞭草烯醇 trans-Verbenol	C ₁₀ H ₁₆ O	20.292	-	0.06	0.04	-	-	0.06	0.13	0.11	0.11	0.19	-	-	0.21	-	醇类 Alcohols
47	2-壬烯醛 2-Nonenal	C ₉ H ₁₆ O	20.563	-	-	-	-	-	-	0.21	-	-	-	0.18	-	-	-	醛类 Aldehydes
48	异胡薄荷醇 Isopulegol	C ₁₀ H ₁₈ O	20.572	-	0.08	-	-	-	-	-	0.16	-	0.28	-	-	0.23	-	醇类 Alcohols
49	3,6-二氢-4-甲基-2-(2-甲基-1-丙烯基)-2H-吡喃 3,6-dihydro-4-methyl-2-(2-methyl-1-propenyl)-2H-Pyran	C ₁₀ H ₁₆ O	20.795	-	-	-	-	-	-	-	0.14	-	0.17	-	-	0.13	-	吡喃类 Pyran
50	反式-2-壬烯醛 trans-2-Nonenal	C ₉ H ₁₆ O	21.381	0.47	0.66	0.43	0.22	0.38	0.40	2.18	1.22	1.75	1.38	1.98	1.97	2.27	-	醛类 Aldehydes
51	反式-β-松油醇 trans-Cyclohexanol,1-methyl-4-(1-methylethenyl)	C ₁₀ H ₁₈ O	21.698	-	-	-	-	-	-	-	-	-	0.14	-	-	-	-	醇类 Alcohols

52	4'-甲基苯乙酮 Ethanone,1-(4methylphenyl)-	C ₉ H ₁₀ O	22.566	0.13	0.22	0.13	-	-	0.04	0.68	-	0.19	0.51	0.37	-	0.47	酮类 Ketones
53	4-异丙基-2-环己烯酮 2-Cyclohexen-1-one, 4-(1-methylethyl)-	C ₉ H ₁₄ O	22.665	0.13	0.15	-	-	-	-	-	0.10	-	0.27	-	-	0.17	酮类 Ketones
54	反式 p-薄荷-1(7),8-二烯-2-醇 trans-p-mentha-1(7),8-dien-2-ol	C ₁₀ H ₁₆ O	22.836	0.28	0.41	0.28	0.13	0.27	0.23	0.80	0.47	0.33	0.82	0.43	0.17	0.72	醇类 Alcohols
55	(1R, 2S, 4R)-2,7,7-三甲基双 环[2.2.1]庚烷-2-醇 (1R,2S,4R)-2,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol	C ₁₀ H ₁₈ O	23.205	-	-	-	-	-	-	-	-	-	-	-	1.37	1.52	醇类 Alcohols
56	α-松油醇 α-Terpineol	C ₁₀ H ₁₈ O	23.249	1.97	1.42	0.79	0.86	0.97	1.09	-	-	-	1.47	1.58	-	-	醇类 Alcohols
57	p-薄荷-1(7),8(10)-二烯-9-醇 p-Mentha-1(7),8(10)-dien-9-ol	C ₁₀ H ₁₆ O	23.387	-	-	-	-	-	-	-	-	-	-	-	0.63	1.26	醇类 Alcohols
58	二氢香芹酮 dihydro-Carvone	C ₁₀ H ₁₆ O	23.651	-	0.07	-	-	-	-	0.11	-	-	-	0.13	-	-	酮类 Ketones
59	癸醛 Decanal	C ₁₀ H ₂₀ O	24.039	0.25	0.28	0.22	0.22	0.19	0.22	0.78	0.55	0.76	0.66	0.96	0.86	0.86	醛类 Aldehydes
60	6,6-二甲基环辛基-2,4-二酮 6,6-Dimethylcycloocta-2,4-dione	C ₁₀ H ₁₄ O	24.130	-	-	-	-	-	-	-	0.21	-	-	-	-	0.37	酮类 Ketones

61	5-异丙烯基-2-甲基环戊-1-烯 羧醛 5-Isopropenyl-2-Methylcyclop ent-1-enecarboxaldehyde	C ₁₀ H ₁₄ O	24.141	-	0.14	-	-	-	-	-	-	-	-	-	-	-	-	醛类 Aldehydes
62	反式-香茅醇 trans-Carveol	C ₁₀ H ₁₆ O	24.517	1.65	2.29	1.46	0.65	1.44	1.12	2.04	2.20	1.43	4.32	1.90	0.78	3.73	醇类 Alcohols	
63	橙花醇 Nerol	C ₁₀ H ₁₈ O	24.893	0.08	-	-	-	-	0.10	-	-	-	-	-	-	-	醇类 Alcohols	
64	马鞭草烯酮 Verbenone	C ₁₀ H ₁₄ O	24.932	-	-	-	-	-	-	-	0.15	-	0.24	-	-	0.38	酮类 Ketones	
65	香芹醇 Carveol	C ₁₀ H ₁₆ O	25.160	0.47	0.47	0.28	0.19	0.30	0.24	0.33	0.27	0.21	0.48	0.39	0.21	0.46	醇类 Alcohols	
66	香芹酮 Carvone*	C ₁₀ H ₁₄ O	25.652	3.41	4.4	2.97	1.34	2.51	2.14	4.58	4.10	3.54	8.07	4.64	2.36	7.73	酮类 Ketones	
67	乙酸芳樟酯 Linalyl acetate*	C ₁₂ H ₂₀ O ₂	26.189	9.06	10.1	6.75	9.34	7.72	8.29	4.79	6.34	3.81	10.97	4.89	2.45	6.50	酯类 Esters	
68	反式-2-癸烯醛 trans-2-Decenal	C ₁₀ H ₁₈ O	26.664	0.31	0.36	-	0.24	-	0.33	1.90	1.15	1.78	1.66	2.06	1.96	2.22	醛类 Aldehydes	
69	(S)-3-甲基-6β-异丙烯-2-环己 烯-1-酮 (S)-3-Methyl-6β-isopropenyl-2 -cyclohexene-1-one	C ₁₀ H ₁₄ O	26.779	-	-	-	-	-	--	-	-	-	0.21	-	-	0.19	酮类 Ketones	
70	2-正己基噻吩 2-hexyl-thiophen	C ₁₀ H ₁₆ S	26.970	-	0.14	-	-	0.11	0.11	-	-	-	-	-	-	-	噻吩类 Thiophene derivatives	

	2-羟基-5-甲基苯乙酮																
71	2-Hydroxy-5-methylacetophenone	C ₉ H ₁₀ O ₂	27.055	-	-	-	-	-	-	0.56	-	-	0.91	0.54	-	1.04	酮类 Ketones
	Z-8-十八碳烯-1-醇乙酸酯																
72	Z-8-Octadecen-1-ol acetate	C ₂₀ H ₃₈ O ₂	27.124	0.18	0.28	0.19	-	-	-	-	-	-	-	-	-	-	酯类 Esters
	香芹酮氧化物																
73	Carvone oxide	C ₁₀ H ₁₄ O ₂	27.132	-	-	-	-	-	-	0.57	-	-	0.54	-	-	0.69	酮类 Ketones
	正壬酸																
74	Nonanoic acid	C ₉ H ₁₈ O ₂	27.370	-	-	-	-	-	-	0.37	-	-	-	0.47	-	-	脂肪酸类 Fatty acids
	己酸戊酯																
75	Hexanoic acid, pentyl ester	C ₁₁ H ₂₂ O ₂	27.893	0.45	0.50	0.36	-	0.38	0.36	1.47	0.70	0.99	0.67	1.16	1.26	0.94	酯类 Esters
	(E,E)-2,4-十二碳二烯醛																
76	(E,E)-2,4-Dodecadienal	C ₁₂ H ₂₀ O	28.043	-	-	-	-	-	-	0.21	-	-	-	-	-	0.27	醛类 Aldehydes
	4-乙基环己醇																
77	4-Ethylcyclohexanol	C ₈ H ₁₆ O	28.046	-	0.11	-	-	0.08	0.04	-	-	0.23	0.22	0.27	-	-	醇类 Alcohols
	紫苏醇																
78	Perycorolle	C ₁₀ H ₁₆ O	28.158	-	0.05	-	-	-	-	-	0.10	-	0.20	-	-	0.20	醇类 Alcohols
	Δ-松油醇																
79	Δ-Terpineol, acetate	C ₁₂ H ₂₀ O ₂	28.778	0.14	0.14	-	0.09	-	-	-	-	-	-	-	-	-	醇类 Alcohols
	(2E,4Z)-2,4-癸二烯醛																
80	(2E,4Z)-2,4-Decadienal	C ₁₀ H ₁₆ O	29.017	0.13	0.26	0.20	0.15	0.19	0.21	0.58	0.49	0.75	0.66	0.81	0.86	0.96	醛类 Aldehydes
	环氧十五烷-2,13-二酮																
81	Oxacyclohexadecane-2,13-dione	C ₁₅ H ₂₆ O ₃	29.718	-	-	-	-	-	-	0.62	-	-	0.26	0.70	-	-	酮类 Ketones
	乙酸松油酯																
82	Terpinyl acetate	C ₁₂ H ₂₀ O ₂	30.091	1.8	1.61	1.08	1.58	1.13	1.46	0.61	0.55	0.44	0.72	0.78	0.35	0.58	酯类 Esters

120	5-十二烷基二氢-2(3H)-呋喃酮 2(3H)-Furanone,5-dodecyldihydro	C ₁₆ H ₃₀ O ₂	41.835	-	-	-	-	-	-	-	0.13	0.12	0.06	-	-	0.09	酮类 Ketones
121	亚油酸 Linoleic acid	C ₁₈ H ₃₂ O ₂	42.340	-	-	0.38	0.48	0.29	0.18	-	0.08	0.07	-	-	0.13	-	脂肪酸类 Fatty acids
122	2-羟基环戊十二酮 2-Hydroxycyclopentadecanone	C ₁₅ H ₂₈ O ₂	42.419	0.11	0.05	2.19	2.27	1.46	1.18	-	1.22	1.02	0.16	-	0.86	0.32	酮类 Ketones
123	硬脂酰胺 Octadecanamide	C ₁₈ H ₃₇ NO	43.242	-	0.10	-	-	-	0.19	0.10	0.20	0.28	0.11	-	0.35	0.12	酰胺类 Amides
124	棕榈油酸辛酯 Octyl palmitoleate	C ₂₄ H ₄₈ O ₂	45.189	0.09	0.06	0.38	0.63	0.29	0.37	-	0.28	0.36	0.08	-	0.63	0.14	酯类 Esters

标有*为经过对照品确认成分，“-”表示未检出或匹配度<80%，标有△为匹配度≥80%但对对照品验证后与数据库鉴定结果不一致的未确认成分

*Indicates components confirmed by reference standard. “-” denotes not detected or match rate <80%. Components marked with △ indicate unconfirmed constituents with a match rate ≥80% but inconsistent with database identification results following reference standard verification