

Supplementary Material

Comparison of Volatile Compositions among Four Related *Ligusticum chuanxiong* Herbs by HS-SPME-GC-MS

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Table S1. Retention time, mass spectrometry detection parameters, and regression equation of standards.

No.	Compound	RT (min)	RI	Quantifier ion (m/z)	Qualifier ion (m/z)	Qualifier ion (m/z)	Regression equation
1	Ethyl acetate	1.95	886	70.00 > 55.00	88.00 > 61.00	70.00 > 43.00	$Y = -0.00006X^2 + 53.35321X + 384.11828$
2	Diacetyl	2.63	960	86.00 > 43.00	43.00 > 15.00	43.00 > 14.00	$Y = -0.00174X^2 + 63.50733X - 2337.63651$
3	Pentanal	2.68	966	86.00 > 58.00	67.00 > 65.00	71.00 > 53.00	$Y = 0.00000X^2 + 4.99306X - 49.83822$
4	sec-Butyl acetate	2.80	979	87.00 > 43.00	56.00 > 41.00	56.00 > 39.00	$Y = -0.00067X^2 + 166.98618X + 383.54682$
5	Methyl methacrylate	2.97	998	69.00 > 41.00	100.00 > 69.00	69.00 > 39.00	$Y = 0.00055X^2 + 79.63112X + 466.35134$
6	alpha-Pinene	3.23	1012	93.00 > 77.00	93.00 > 51.00	136.00 > 93.00	$Y = 0.00044X^2 + 722.66259X + 153.40652$
7	Toluene	3.48	1025	91.00 > 65.00	91.00 > 39.00	65.00 > 39.00	$Y = -0.00196X^2 + 570.17276X + 4048.73940$
8	Ethyl-2-methylbutyrate	3.76	1039	102.00 > 74.00	115.00 > 87.00	102.00 > 56.00	$Y = 0.00772X^2 + 362.20906X + 2558.71661$
9	Dimethyl disulfide	4.09	1056	94.00 > 79.00	94.00 > 61.00	79.00 > 64.00	$Y = 0.00024X^2 + 282.67510X - 306.58905$
10	n-Butyl acetate	4.15	1059	73.00 > 43.00	61.00 > 43.00	73.00 > 55.00	$Y = -0.00011X^2 + 177.75053X + 1152.35484$
11	2-Hexanone	4.23	1063	100.00 > 85.00	100.00 > 71.00	85.00 > 57.00	$Y = 0.00048X^2 + 58.20824X + 2892.35270$
12	Hexanal	4.33	1068	56.00 > 41.00	82.00 > 67.00	56.00 > 39.00	$Y = 0.00022X^2 + 92.11251X + 1249.76336$
13	beta-Pinene	4.89	1097	93.00 > 91.00	93.00 > 77.00	93.00 > 51.00	$Y = 0.00265X^2 + 374.60702X + 625.10567$
14	Ethylbenzene	5.39	1117	106.00 > 91.00	91.00 > 65.00	106.00 > 65.00	$Y = 0.00262X^2 + 909.46352X + 1195.16531$
15	5-Hexene-2-one	5.49	1121	98.00 > 43.00	83.00 > 55.00	98.00 > 83.00	$Y = -0.00034X^2 + 57.29575X - 160.43427$
16	Mesityl oxide	5.49	1121	98.00 > 83.00	83.00 > 55.00	98.00 > 55.00	$Y = 0.00203X^2 + 403.80718X - 29.11896$
17	p-Xylene	5.57	1124	106.00 > 91.00	91.00 > 65.00	91.00 > 39.00	$Y = 0.00003X^2 + 755.45782X + 643.13703$
18	m-Xylene	5.72	1130	106.00 > 91.00	91.00 > 65.00	91.00 > 39.00	$Y = 0.00220X^2 + 640.88871X + 2454.22435$

19	3-Heptanone	6.11	1145	85.00 > 57.00	85.00 > 41.00	114.00 > 85.00	$Y = -0.00048X^2 + 190.87646X - 20.43927$
20	o-Xylene	6.78	1171	106.00 > 91.00	91.00 > 65.00	106.00 > 65.00	$Y = 0.00218X^2 + 572.02237X + 2534.97346$
21	2-Heptanone	6.80	1172	71.00 > 43.00	114.00 > 85.00	71.00 > 41.00	$Y = 0.00162X^2 + 199.00709X + 1415.01346$
22	Limonene	7.19	1187	136.00 > 93.00	107.00 > 91.00	107.00 > 65.00	$Y = 0.00031X^2 + 82.97084X - 36.39870$
23	Eucalyptol	7.42	1196	139.00 > 43.00	154.00 > 139.00	154.00 > 125.00	$Y = 0.00025X^2 + 43.29709X - 115.35588$
24	Diethyl disulfide	7.50	1199	122.00 > 94.00	94.00 > 66.00	122.00 > 66.00	$Y = 0.00267X^2 + 439.31271X + 362.19506$
25	1-Methoxy-2-propyl acetate	7.88	1217	87.00 > 43.00	72.00 > 57.00	72.00 > 29.00	$Y = 0.00023X^2 + 96.04189X + 348.61555$
26	1-Pentanol	8.43	1243	70.00 > 55.00	55.00 > 53.00	70.00 > 53.00	$Y = 0.00230X^2 + 189.23376X + 562.80790$
27	Styrene	8.45	1244	104.00 > 78.00	78.00 > 52.00	104.00 > 52.00	$Y = -0.00062X^2 + 749.04325X + 1683.15989$
28	2-Methylpyrazine	8.58	1250	94.00 > 67.00	67.00 > 40.00	94.00 > 40.00	$Y = -0.00067X^2 + 362.01027X - 741.13353$
29	n-Hexyl acetate	8.92	1266	69.00 > 41.00	84.00 > 55.00	84.00 > 69.00	$Y = 0.00104X^2 + 118.46377X + 1709.11496$
30	Acetoin	8.96	1268	45.00 > 43.00	88.00 > 45.00	45.00 > 27.00	$Y = -0.00004X^2 + 22.98718X + 1455.64001$
31	2-Octanone	9.13	1276	128.00 > 85.00	128.00 > 57.00	128.00 > 72.00	$Y = 0.00004X^2 + 37.92409X - 195.43302$
32	Octanal	9.21	1280	84.00 > 55.00	100.00 > 82.00	84.00 > 69.00	$Y = -0.00001X^2 + 14.63760X + 749.42123$
33	2-Ethoxyethyl acetat	9.34	1286	72.00 > 44.00	88.00 > 61.00	72.00 > 42.00	$Y = 0.00037X^2 + 325.41558X + 1776.95653$
34	trans-2-Heptenal	9.78	1308	83.00 > 55.00	83.00 > 53.00	112.00 > 83.00	$Y = 0.00011X^2 + 14.93439X + 258.73876$
35	5-Nonanone	9.92	1316	85.00 > 57.00	142.00 > 100.00	85.00 > 41.00	$Y = 0.00081X^2 + 325.93916X + 1435.98471$
36	2-Ethylpyrazine	9.96	1318	107.00 > 79.00	107.00 > 52.00	80.00 > 53.00	$Y = 0.00048X^2 + 281.97793X + 129.57937$
37	alpha-Methylstyren	9.97	1319	103.00 > 77.00	118.00 > 91.00	103.00 > 51.00	$Y = 0.00430X^2 + 393.09476X + 420.74097$
38	2,3-Dimethylpyrazine	10.19	1331	108.00 > 67.00	108.00 > 81.00	108.00 > 93.00	$Y = 0.00032X^2 + 447.59481X + 450.08392$
39	2-n-Propylpyridine	10.62	1355	93.00 > 66.00	106.00 > 78.00	93.00 > 78.00	$Y = 0.00011X^2 + 225.47371X - 205.79265$
40	Dimethyl trisulfide	10.79	1365	126.00 > 79.00	126.00 > 61.00	79.00 > 64.00	$Y = 0.00348X^2 + 288.41210X + 257.03082$
41	2-Nonanone	11.02	1378	71.00 > 43.00	142.00 > 99.00	71.00 > 41.00	$Y = 0.00068X^2 + 70.23745X + 690.59533$
42	Butyl cellosolve	11.22	1389	87.00 > 57.00	100.00 > 72.00	87.00 > 45.00	$Y = 0.00120X^2 + 151.47935X + 615.53002$
43	5-Ethyl-2-methylpyridine	11.40	1399	106.00 > 77.00	121.00 > 106.00	106.00 > 79.00	$Y = 0.00136X^2 + 624.10051X + 454.87175$
44	1,2,4,5-Tetramethylbenzene	11.56	1409	119.00 > 91.00	134.00 > 119.00	119.00 > 77.00	$Y = 0.00146X^2 + 478.93180X - 376.59810$
45	2-Isopropyl-3-methoxypyrazine	11.81	1425	152.00 > 137.00	137.00 > 109.00	152.00 > 124.00	$Y = 0.00109X^2 + 216.81741X + 108.85579$
46	p-Dichlorobenzene	11.88	1430	146.00 > 111.00	146.00 > 75.00	111.00 > 75.00	$Y = 0.00134X^2 + 455.30500X + 2316.56221$
47	Acetic acid (ethylic acid)	11.95	1434	60.00 > 43.00	60.00 > 42.00	60.00 > 45.00	$Y = 0.00404X^2 - 1.43486X + 891.96944$
48	trans, trans-2,4-Heptadienal	12.65	1479	110.00 > 81.00	81.00 > 53.00	81.00 > 27.00	$Y = 0.00066X^2 + 109.85850X - 12.62340$
49	2-Ethyl-1-hexanol	12.65	1479	83.00 > 55.00	98.00 > 56.00	83.00 > 41.00	$Y = 0.00046X^2 + 282.36863X + 76.03495$
50	n-Decanal	12.83	1491	112.00 > 70.00	112.00 > 55.00	112.00 > 83.00	$Y = 0.00018X^2 + 23.24599X - 23.56368$
51	Ethyl sorbate	12.88	1494	95.00 > 67.00	140.00 > 97.00	95.00 > 65.00	$Y = 0.00142X^2 + 295.94846X - 33.66240$

52	Camphor	13.01	1503	95.00 > 55.00	152.00 > 108.00	95.00 > 67.00	$Y = 0.00061X^2 + 112.89822X + 362.62820$
53	Benzaldehyde	13.04	1505	105.00 > 77.00	106.00 > 77.00	77.00 > 51.00	$Y = 0.00112X^2 + 452.45632X - 221.75106$
54	2-Nonanol	13.08	1508	69.00 > 41.00	98.00 > 56.00	69.00 > 39.00	$Y = 0.00067X^2 + 144.79292X + 272.95999$
55	2-Isobutyl-3-methox pyrazine	13.18	1515	124.00 > 94.00	124.00 > 81.00	124.00 > 79.00	$Y = 0.00387X^2 + 568.30547X - 209.54844$
56	Propionic acid	13.23	1518	74.00 > 56.00	74.00 > 46.00	57.00 > 29.00	$Y = 0.00247X^2 + 7.69775X + 190.06633$
57	2-Nonenal	13.32	1525	83.00 > 55.00	96.00 > 81.00	83.00 > 29.00	$Y = 0.00071X^2 + 67.09127X - 45.02346$
58	3-Ethyl-4- methylpyridine	13.42	1532	106.00 > 77.00	121.00 > 106.00	106.00 > 79.00	$Y = 0.00455X^2 + 496.45728X - 2525.94234$
59	Linalool	13.48	1536	93.00 > 77.00	121.00 > 93.00	93.00 > 51.00	$Y = 0.00138X^2 + 165.64341X + 1676.68207$
60	1-Octanol	13.62	1546	69.00 > 41.00	84.00 > 55.00	84.00 > 69.00	$Y = 0.00082X^2 + 143.52175X + 1878.99309$
61	Isobutyric acid	13.69	1551	73.00 > 55.00	88.00 > 73.00	73.00 > 27.00	$Y = 0.00000X^2 + 84.02110X - 46524.04564$
62	5-Methyl furfural	13.77	1557	110.00 > 53.00	81.00 > 53.00	110.00 > 81.00	$Y = 0.00064X^2 + 100.58536X - 209.96922$
63	Isophorone	14.04	1576	82.00 > 54.00	138.00 > 82.00	82.00 > 39.00	$Y = -0.00080X^2 + 357.08990X - 174.62370$
64	2-Methylisoborneol	14.14	1583	95.00 > 55.00	95.00 > 67.00	95.00 > 41.00	$Y = -0.00000X^2 + 202.42463X + 461.46943$
65	2-Undecanone	14.21	1588	71.00 > 43.00	170.00 > 85.00	71.00 > 41.00	$Y = 0.00009X^2 + 79.13147X + 1144.77407$
66	Butyric acid	14.51	1610	60.00 > 42.00	73.00 > 55.00	60.00 > 45.00	$Y = 0.00944X^2 + 90.59351X - 4106.39202$
67	Benzyl mercaptan	14.55	1613	124.00 > 91.00	91.00 > 65.00	91.00 > 39.00	$Y = 0.00426X^2 + 292.02974X - 5326.23324$
68	Phenylacetaldehyde	14.73	1627	91.00 > 65.00	120.00 > 91.00	91.00 > 39.00	$Y = -0.00593X^2 + 190.36466X - 774.65598$
69	L-Menthol	14.75	1628	95.00 > 67.00	138.00 > 95.00	95.00 > 55.00	$Y = -0.00029X^2 + 64.41132X - 516.71784$
70	Acetophenone	14.82	1634	105.00 > 77.00	120.00 > 105.00	105.00 > 51.00	$Y = 0.00219X^2 + 683.24573X + 382.02616$
71	trans-2-Decenal	14.84	1635	107.00 > 79.00	107.00 > 91.00	121.00 > 93.00	$Y = 0.00010X^2 + 13.72079X + 79.61158$
72	Verbenol	14.98	1646	119.00 > 91.00	119.00 > 117.00	119.00 > 77.00	$Y = 0.00014X^2 + 27.92801X - 148.95612$
73	Isovaleric acid	15.06	1652	60.00 > 42.00	87.00 > 69.00	60.00 > 45.00	$Y = 0.00670X^2 + 117.37406X - 9871.91958$
74	2-Methyl butyric aci	15.09	1654	74.00 > 56.00	87.00 > 69.00	87.00 > 59.00	$Y = 0.00231X^2 + 30.96562X - 2547.40212$
75	Salicylaldehyde	15.20	1663	122.00 > 65.00	122.00 > 93.00	104.00 > 76.00	$Y = 0.00122X^2 + 150.71498X - 328.20840$
76	alpha-Terpineol	15.50	1686	136.00 > 121.00	121.00 > 93.00	136.00 > 93.00	$Y = 0.00051X^2 + 95.13289X - 32.40006$
77	trans, trans-2,4- Nonadienal	15.56	1690	81.00 > 53.00	138.00 > 81.00	81.00 > 27.00	$Y = 0.02555X^2 + 119.63726X - 471.69438$
78	Borneol	15.57	1691	95.00 > 67.00	139.00 > 95.00	95.00 > 55.00	$Y = 0.00084X^2 + 253.71772X + 198.14530$
79	Verbenone	15.57	1691	107.00 > 91.00	150.00 > 107.00	107.00 > 65.00	$Y = 0.00070X^2 + 134.49475X + 155.39405$
80	n-Dodecanal	15.70	1701	110.00 > 67.00	140.00 > 70.00	110.00 > 81.00	$Y = 0.00019X^2 + 6.50905X - 262.14594$
81	p-Dibromobenzene	15.85	1713	236.00 > 155.00	236.00 > 157.00	155.00 > 76.00	$Y = 0.00038X^2 + 215.48270X + 330.14399$
82	n-Valeric acid	15.92	1719	60.00 > 42.00	73.00 > 55.00	60.00 > 45.00	$Y = 0.00580X^2 + 56.42323X - 4438.38744$
83	Naphthalene	16.01	1726	128.00 > 102.00	128.00 > 78.00	102.00 > 76.00	$Y = 0.00106X^2 + 476.73953X + 875.81149$
84	6-Chloro-o-cresol	16.35	1754	107.00 > 77.00	142.00 > 107.00	107.00 > 79.00	$Y = 0.00153X^2 + 331.12314X + 226.46380$

85	Methyl salicylate	16.46	1763	120.00 > 92.00	152.00 > 120.00	120.00 > 64.00	$Y = 0.00140X^2 + 649.86946X + 286.50910$
86	Isocaproic acid	16.73	1785	83.00 > 55.00	74.00 > 56.00	101.00 > 55.00	$Y = 0.00000X^2 + 33.52523X - 17021.39256$
87	trans, trans-2,4-Decadienal	16.90	1799	81.00 > 53.00	152.00 > 81.00	81.00 > 79.00	$Y = 0.00234X^2 + 185.52948X + 689.40595$
88	2,4,6-Trichloroanisole	16.90	1799	195.00 > 167.00	210.00 > 195.00	210.00 > 167.00	$Y = 0.00080X^2 + 382.35100X + 173.53273$
89	Geosmin	17.13	1818	112.00 > 97.00	112.00 > 83.00	112.00 > 69.00	$Y = 0.00148X^2 + 497.14002X + 335.63368$
90	Caproic acid	17.21	1825	73.00 > 55.00	87.00 > 45.00	73.00 > 27.00	$Y = 0.00421X^2 + 120.72779X - 8229.23458$
91	o-Chlorophenol	17.30	1833	128.00 > 64.00	128.00 > 92.00	100.00 > 65.00	$Y = 0.00038X^2 + 547.76634X - 393.94397$
92	Geraniol	17.30	1833	69.00 > 41.00	69.00 > 39.00	123.00 > 81.00	$Y = 0.01126X^2 + 481.16604X + 49.10674$
93	2-Methylnaphthalene	17.37	1839	142.00 > 115.00	115.00 > 89.00	115.00 > 63.00	$Y = 0.00191X^2 + 387.77246X + 765.02439$
94	Guaiacol	17.41	1842	124.00 > 109.00	109.00 > 81.00	124.00 > 81.00	$Y = 0.00435X^2 + 429.74353X + 2319.99279$
95	Benzyl acetone	17.42	1843	148.00 > 105.00	148.00 > 133.00	105.00 > 77.00	$Y = 0.00042X^2 + 211.07584X + 268.35891$
96	alpha-Ionone	17.42	1843	121.00 > 77.00	192.00 > 177.00	121.00 > 91.00	$Y = 0.00097X^2 + 263.46627X + 1033.71227$
97	1-Undecanol	17.53	1853	83.00 > 55.00	111.00 > 69.00	83.00 > 41.00	$Y = 0.00123X^2 + 152.80585X + 224.52339$
98	Benzyl alcohol	17.58	1857	108.00 > 79.00	79.00 > 51.00	108.00 > 77.00	$Y = 0.00127X^2 + 292.10822X + 264.65797$
99	1-Methylnaphthalene	17.79	1875	142.00 > 115.00	115.00 > 89.00	115.00 > 65.00	$Y = 0.00029X^2 + 436.21687X - 898.91599$
100	2,4-Dichloroanisole	17.92	1886	161.00 > 133.00	176.00 > 161.00	176.00 > 133.00	$Y = 0.00036X^2 + 412.41081X + 87.01309$
101	2-Phenylethanol	18.00	1893	91.00 > 65.00	122.00 > 92.00	91.00 > 63.00	$Y = -0.00189X^2 + 500.63206X + 1658.75907$
102	gamma-Octalactone	18.06	1898	85.00 > 57.00	100.00 > 72.00	100.00 > 58.00	$Y = -0.00045X^2 + 319.60206X + 475.52903$
103	Dibutylhydroxytoluene	18.09	1901	220.00 > 205.00	205.00 > 177.00	205.00 > 145.00	$Y = 0.00562X^2 + 380.74561X + 677.02438$
104	beta-Ionone	18.38	1927	177.00 > 162.00	177.00 > 147.00	192.00 > 177.00	$Y = 0.00148X^2 + 212.24615X + 22.20561$
105	Enanthic acid	18.44	1932	87.00 > 59.00	101.00 > 55.00	87.00 > 45.00	$Y = 0.00000X^2 + 51.44300X - 19843.59104$
106	Benzothiazole	18.54	1941	135.00 > 108.00	108.00 > 69.00	135.00 > 91.00	$Y = 0.00373X^2 + 624.95387X + 657.12157$
107	o-Bromophenol	18.63	1949	172.00 > 65.00	174.00 > 65.00	172.00 > 93.00	$Y = 0.02413X^2 + 297.69408X + 28.30057$
108	1-Dodecanol	18.70	1955	111.00 > 69.00	111.00 > 55.00	125.00 > 69.00	$Y = -0.00001X^2 + 74.07051X + 265.72713$
109	o-Cresol	18.97	1980	108.00 > 77.00	108.00 > 79.00	90.00 > 63.00	$Y = -0.00036X^2 + 170.18051X + 38.65421$
110	Phenol	19.01	1983	94.00 > 66.00	66.00 > 40.00	94.00 > 40.00	$Y = 0.00211X^2 + 230.01969X + 4074.64719$
111	4,5-Epoxy-(E)-2-decenal	19.09	1990	81.00 > 53.00	152.00 > 81.00	81.00 > 79.00	$Y = -0.00041X^2 + 13.93196X + 187.26731$
112	Methyleugenol	19.14	1995	178.00 > 107.00	178.00 > 163.00	147.00 > 91.00	$Y = 0.00150X^2 + 220.61849X + 24.01496$
113	p-Ethylguaiacol	19.32	2012	152.00 > 137.00	137.00 > 122.00	137.00 > 94.00	$Y = 0.00111X^2 + 387.81029X - 602.84119$
114	Caprylic acid	19.60	2038	101.00 > 55.00	115.00 > 45.00	101.00 > 45.00	$Y = 0.00000X^2 + 35.74939X - 19007.17973$
115	2-Bromo-p-cresol	19.61	2039	186.00 > 107.00	188.00 > 107.00	186.00 > 77.00	$Y = 0.00066X^2 + 190.17871X - 357.75705$
116	4,6-Dichloro-o-cresol	19.76	2053	141.00 > 77.00	176.00 > 141.00	176.00 > 77.00	$Y = 0.00123X^2 + 358.40677X + 308.74022$
117	p-Cresol	19.82	2059	107.00 > 77.00	77.00 > 51.00	107.00 > 51.00	$Y = 0.00145X^2 + 397.82831X + 865.85430$

118	m-Cresol	19.91	2067	108.00 > 77.00	108.00 > 79.00	108.00 > 90.00	$Y = 0.00017X^2 + 114.43044X + 162.84114$
119	2,6-Dichlorophenol	20.15	2090	162.00 > 63.00	162.00 > 98.00	164.00 > 63.00	$Y = 0.00185X^2 + 254.67861X - 439.17762$
120	2-Phenoxyethanol	20.47	2121	94.00 > 66.00	138.00 > 94.00	94.00 > 55.00	$Y = -0.00181X^2 + 357.54980X + 595.11035$
121	2,3-Xylenol	20.51	2125	122.00 > 107.00	107.00 > 77.00	107.00 > 79.00	$Y = -0.00030X^2 + 671.89159X - 557.60754$
122	gamma-Decalactone	20.54	2128	85.00 > 57.00	128.00 > 95.00	128.00 > 71.00	$Y = 0.00186X^2 + 243.51083X + 1817.81703$
123	Pelargonic acid	20.72	2145	129.00 > 87.00	115.00 > 69.00	115.00 > 45.00	$Y = 0.00569X^2 + 36.80456X - 2769.12181$
124	Bis(2-methyl-3-furyl)disulfide	20.72	2145	226.00 > 113.00	113.00 > 85.00	113.00 > 45.00	$Y = 0.00571X^2 + 317.05581X - 40.29907$
125	Eugenol	20.76	2149	164.00 > 149.00	164.00 > 131.00	149.00 > 121.00	$Y = 0.00128X^2 + 151.73916X - 109.38319$
126	p-Ethylphenol	20.78	2151	107.00 > 77.00	122.00 > 107.00	107.00 > 51.00	$Y = -0.00107X^2 + 561.90309X + 505.05426$
127	2,4-Dichlorophenol	20.83	2156	162.00 > 98.00	162.00 > 126.00	126.00 > 98.00	$Y = 0.00199X^2 + 168.44271X + 206.18320$
128	1-Tetradecanol	20.85	2158	111.00 > 69.00	111.00 > 41.00	168.00 > 55.00	$Y = 0.00142X^2 + 76.08629X + 3337.00972$
129	Caprolactam	20.90	2163	113.00 > 85.00	85.00 > 67.00	113.00 > 56.00	$Y = 0.00141X^2 + 107.49736X - 3501.08451$
130	2,4,6-Trichloroanilin	21.04	2177	195.00 > 124.00	195.00 > 159.00	159.00 > 124.00	$Y = 0.00060X^2 + 179.14664X - 12.33645$
131	p-Propylphenol	21.67	2240	107.00 > 77.00	136.00 > 107.00	107.00 > 51.00	$Y = -0.00009X^2 + 723.82969X + 131.42431$
132	Capric acid	21.76	2249	129.00 > 87.00	143.00 > 87.00	129.00 > 59.00	$Y = 0.00532X^2 + 69.44105X - 2228.78530$
133	2,4,6-Tribromoanisole	22.00	2274	344.00 > 329.00	344.00 > 301.00	301.00 > 141.00	$Y = 0.00082X^2 + 154.14394X - 114.31777$
134	2,4,6-Trichlorophenol	22.46	2321	132.00 > 97.00	196.00 > 97.00	196.00 > 132.00	$Y = 0.00582X^2 + 131.40869X + 91.37197$
135	Isoeugenol	22.50	2326	164.00 > 149.00	164.00 > 131.00	149.00 > 121.00	$Y = 0.00035X^2 + 77.90550X - 246.72900$
136	2,4-Dibromophenol	22.61	2337	252.00 > 63.00	250.00 > 63.00	250.00 > 143.00	$Y = 0.00063X^2 + 54.36920X - 453.15893$
137	gamma-Dodecalactone	22.85	2363	85.00 > 57.00	128.00 > 95.00	85.00 > 29.00	$Y = 0.00007X^2 + 233.95008X + 107.90282$
138	Indole	23.42	2424	117.00 > 90.00	90.00 > 63.00	117.00 > 64.00	$Y = 0.00581X^2 + 837.96570X + 4865.08467$
139	Coumarin	23.49	2432	146.00 > 118.00	118.00 > 90.00	146.00 > 90.00	$Y = 0.00098X^2 + 654.98572X - 150.50469$
140	2,6-Dibromo-p-cresol	23.54	2437	266.00 > 185.00	264.00 > 185.00	266.00 > 187.00	$Y = -0.00001X^2 + 116.62962X - 830.65430$
141	2,6-Dibromophenol	23.58	2442	252.00 > 63.00	250.00 > 143.00	252.00 > 143.00	$Y = 0.00033X^2 + 101.13422X - 277.15891$
142	p-Bromoxylenol	23.60	2444	200.00 > 121.00	202.00 > 121.00	202.00 > 77.00	$Y = -0.00042X^2 + 218.40862X - 31.25234$
143	Lauric acid	23.75	2461	157.00 > 87.00	200.00 > 87.00	157.00 > 59.00	$Y = 0.00178X^2 + 11.89069X - 603.66362$
144	Benzophenone	23.82	2468	105.00 > 77.00	182.00 > 105.00	105.00 > 51.00	$Y = 0.00747X^2 + 816.90080X + 8396.68133$
145	Skatole	23.85	2472	130.00 > 77.00	130.00 > 103.00	103.00 > 77.00	$Y = 0.00539X^2 + 603.11259X + 2224.83764$
146	Butylphthalide	24.33	2525	159.00 > 103.10	159.00 > 77.10	159.00 > 131.10	$Y = -0.00180X^2 + 336.99437X + 3518.66463$
147	Phenylacetic acid	24.39	2532	136.00 > 91.00	91.00 > 65.00	91.00 > 63.00	$Y = 0.00000X^2 + 227.65932X - 144667.90429$
148	Vanillin	24.42	2536	152.00 > 123.00	123.00 > 108.00	152.00 > 109.00	$Y = 0.00058X^2 + 126.15172X - 1012.41133$
149	Ligustilide	24.83	2582	190.00 > 148.10	148.00 > 105.10	148.00 > 78.10	$Y = -0.00121X^2 + 211.16532X + 487.55948$
150	Senkyunolide A	25.10	2613	107.00 > 77.10	107.00 > 79.10	107.00 > 51.10	$Y = -0.00267X^2 + 394.57229X + 2952.20964$

151	3-Butylidenephthalide	25.26	2630	159.00 > 103.10	159.00 > 77.10	159.00 > 131.10	$Y = -0.00012X^2 + 23.15402X + 605.10838$
152	2,4,6-Tribromophenol	26.74	2782	332.00 > 143.00	330.00 > 141.00	332.00 > 222.00	$Y = 0.00029X^2 + 12.93600X - 98.69160$
153	Cinnamic acid	27.20	2823	147.00 > 91.00	103.00 > 77.00	147.00 > 103.00	$Y = 0.00000X^2 + 42.50400X + 0.00000$
154	Dibenzyl disulfide	29.85	3018	91.00 > 65.00	246.00 > 91.00	181.00 > 166.00	$Y = 0.00633X^2 + 889.40870X + 1185.28612$

RT, Retention time; RI, Retention index.

Table S2. N-alkane reference and test data.

No.	Name	Retention time (min)	Test retention time (min)	Reference ion (m/z)	Test ion (m/z)	Peak area ($\mu V \cdot s$)
1	C9	2.201	2.093	128.2	128.2	10862
2	C10	3.200	3.010	142.2	142.2	10780
3	C11	5.332	4.986	156.2	156.2	9941
4	C12	7.831	7.550	170.2	170.2	9013
5	C13	9.895	9.663	184.2	184.2	7074
6	C14	11.649	11.438	198.2	198.2	7559
7	C15	13.192	12.996	212.2	212.2	6020
8	C16	14.594	14.409	226.3	226.3	6333
9	C17	15.895	15.717	240.3	240.3	6926
10	C18	17.119	16.951	254.3	254.3	6188
11	C19	18.280	18.118	268.3	268.3	5250
12	C20	19.385	19.236	282.3	282.3	4239
13	C21	20.442	20.301	296.3	296.3	4428
14	C22	21.453	21.324	310.3	310.3	3230
15	C23	22.424	22.307	324.4	324.4	3285
16	C24	23.359	23.251	338.4	338.4	2945
17	C25	24.258	24.163	352.4	352.4	2635
18	C26	25.127	25.041	366.4	366.4	2184
19	C27	26.055	25.965	380.4	380.4	1662
20	C28	27.112	27.004	394.5	394.5	1797
21	C29	28.354	28.231	408.4	408.4	2154
22	C30	29.849	29.717	422.5	422.5	1394