Electronic Supplementary Material (ESI) for Analytical Methods.

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Table S1. Analysis conditions.

GC-IMS unit	
Analysis time	20min
Chromatographic column type	MXT-5 15m ID:0.53mm
Column temperature	60℃
Carrier/drift gas	N2
IMS temperature	45 ℃
Automatic headspace injection unit	
Injection volume	100ul
Incubation time	15min
Incubation temperature	60℃
Injector needle temperature	65℃
Rotation speed of incubation	500 rpm

Table S2. Gas chromatographic conditions.

Time	E1	E2	R
00:00,000	150mL/min	2ml/min	rec
02:00,000	150mL/min	2ml/min	-
20:00,000	150mL/min	100ml/min	Stop

Table S3. HS-GC-IMS analysis results.

No	Compound	CAS#	Formula	G1	G1	G1	G2	G2	G2	G3	G3	G3	G4	G4	G4	G5	G5	G5	G6	G6	G6
1	Isoeugenol	C97541	C10H12O2	2722.857	2438.38	2341.643	681.463	635.358	557.416	1709.289	1827.028	1993.466	754.59	662.888	629.062	1910.442	1932.24	2016.282	1210.467	1174.144	1028.283
2	4-Ethylphenol	C123079	C8H10O	4079.294	4409.911	4164.636	642.539	627.165	497.804	1419.6	1340.31	1408.438	527.367	449.745	418.593	2436.537	2069.825	2283.288	840.053	814.944	753.226
3	Diallyldisulfide	C2179579	C6H10S2	13583.332	13377.431	13533.322	12304.182	12252.595	11350.821	16843.685	16797.009	16751.1	11801.857	10843.552	10825.31	16662.798	17060.485	16869.397	13985.681	14012.021	13762.223
4	1	unidentified	*	1020.128	1183.499	1141.704	106.62	87.436	90.986	1155.188	1042.227	941.84	71.475	77.34	58.653	1237.645	1187.819	1316.171	92.679	81.495	72.55
5	2	unidentified	*	42.644	63.009	57.607	23.774	11.092	23.289	94.38	72.02	57.166	23.914	17.776	10.252	102.392	92.432	109.548	31.561	11.073	21.465
6	3	unidentified	*	153.966	143.939	167.469	18.198	9.535	18.95	139.216	124.098	114.582	33.442	17.814	11.4	1502.224	1341.74	1452.973	22.239	9.126	17.874
7	1-Octen-3-ol	C3391864	C8H16O	209.025	187.104	245.234	50.505	43.377	50.52	216.188	160.487	166.048	52.823	40.982	39.092	234.674	254.994	240.476	59.215	54.717	61.413
8	(E,E)-2,4-Heptadienal	C4313035	C7H10O	75.773	112.422	142.442	61.794	44.811	43.789	232.07	199.709	223.445	40.671	36.909	27.533	543.088	466.956	393.633	49.648	40.186	43.326
9	4	unidentified	*	2461.646	2578.094	2451.896	2549.492	2642.295	2403.535	3243.262	3228.385	3188.304	2750.819	2323.744	2393.588	3245.181	3309.462	3385.618	3075.768	3193.011	2978.733
10	5	unidentified	*	50.225	54.98	56.725	21.037	15.682	19.568	768.325	696.26	967.866	18.014	61.68	61.137	418.266	465.723	586.804	23.397	18.442	29.141
11	2,5-Dimethylpyrazine	C123320	C6H8N2	173.578	132.485	214.364	14.131	6.033	17.554	199.297	187.849	173.112	19.105	13.015	6.788	228.118	235.423	170.311	15.755	5.507	16.774
12	6	unidentified	*	16.396	19.758	27.26	9.83	6.629	17.195	239.134	182.339	197.435	11.651	13.421	7.277	298.298	273.173	272.687	12.25	5.732	13.129
13	3,4-Dimethylthiophene	C632155	C6H8S	406.156	378.991	389.268	84.15	78.12	49.347	2031.847	2069.077	2090.557	66.983	246.185	263.263	2183.269	2320.185	2425.584	100.33	101.485	85.765
14	(Z)-3-Hexen-1-ol	C928961	C6H12O	1833.143	1583.646	2089.828	918.44	999.535	587.997	5382.589	5959.071	5906.898	564.908	404.709	432.011	4820.793	4890.539	4943.292	806.938	855.333	811.829
15	(E)-2-Hexenal	C6728263	C6H10O	15.809	12.536	16.517	30.188	25.649	31.013	53.81	54.945	78.117	29.005	26.791	25.192	87.741	76.632	135.273	25.052	23.292	26.867
16	Furfuryl Alcohol	C98000	C5H6O2	33.68	77.8	104.479	56.541	54.079	25.693	132.491	196.407	213.333	37.268	37.468	35.444	201.416	265.665	299.205	41.537	40.76	30.524
17	Butylacetate-M	C123864	C6H12O2	11.464	15.362	16.751	12.082	10.204	11.08	120.479	148.269	165.48	22.835	11.305	8.368	287.342	255.13	300.55	11.368	7.432	14.642
18	Butylacetate-D	C123864	C6H12O2	6.775	8.647	6.994	8.472	3.955	7.971	27.489	33.696	55.91	8.91	8.958	4.323	218.522	128.882	185.882	8.634	3.949	10.382
19	7	unidentified	*	28.96	45.794	65.822	37.518	35.228	26.8	122.344	167.773	192.877	41.75	24.507	23.121	226.779	159.184	188.883	29.49	24.523	29.433
20	Hexanal-D	C66251	C6H12O	7.461	8.111	10.154	78.951	87.601	32.193	35.168	79.976	101.999	155.174	16.59	13.912	120.454	55.24	97.587	18.318	15.873	31.063
21	8	unidentified	*	87.734	88.93	89.044	28.053	26.556	32.136	75.56	76.851	86.805	33.141	40.04	39.26	116.688	115.873	120.853	39.085	36.513	36.484
22	3-Methylthiophene	C616444	C5H6S	33.157	31.695	42.996	35.536	36.392	31.834	63.297	94.154	108.295	50.584	51.574	51.624	593.313	723.777	956.022	52.427	49.915	43.364
23	9	unidentified	*	171.602	185.968	178.584	65.876	60.132	47.64	206.031	260.047	280.17	76.747	85.048	80.093	340.816	334.557	363.597	75.725	77.146	50.362
24	10	unidentified	*	82.158	89.184	143.447	20.954	13.186	18.22	316.521	344.47	435.052	26.559	20.025	16.212	1491.37	855.523	1103.929	29.804	22.62	26.718
25	Dimethyl Disulfide	C624920	C2H6S2	23.885	22.616	27.254	82.485	93.45	29.474	73.308	95.687	69.889	118.408	41.969	48.706	261.972	195.541	294.711	204.553	253.627	142.943
26	11	unidentified	*	12.98	11.165	12.035	6.563	3.784	6.455	20.834	31.552	31.048	8.412	6.518	3.825	43.406	30.848	37.94	12.244	7.204	8.358
27	Propylacetate-D	C109604	C5H10O2	33.991	50.815	57.838	35.479	25.75	25.76	1575.101	2206.205	2520.633	27.136	1070.166	1192.558	1549.455	1566.175	1778.959	278.038	329.197	56.481

28	2-Ethylfuran	C3208160	C6H8O	438.596	332.438	465.589	234.411	297.806	43.469	1238.114	1979.772	1851.833	63.291	897.847	998.241	1448.821	1559.228	1624.343	159.393	182.834	114.906
29	12	unidentified	*	20.735	27.428	20.009	12.412	5.824	11.844	71.494	22.334	30.274	10.306	16.101	11.295	647.389	355.445	274.565	13.376	9.694	11.051
30	Hexanal-M	C66251	C6H12O	22.489	23.413	26.315	310.374	322.269	229.225	82.834	151.006	137.56	422.073	133.291	143.441	57.835	65.775	91.985	141.747	154.194	207.855
31	13	unidentified	*	85.013	80.191	81.971	62.152	57.407	49.271	81.619	146.499	137.008	56.42	130.677	135.429	60.706	67.399	73.6	63.351	60.538	46.134
32	Propylacetate-M	C109604	C5H10O2	78.393	97.482	90.269	86.954	95.014	32.437	360.431	413.017	406.647	50.72	593.535	614.302	208.099	259.666	275.821	364.384	389.052	137.709
33	1-Propene-1-methylthio	R301790	C4H8S	2115.124	2405.67	1581.071	1194.099	1276.194	945.646	1136.613	1706.618	1587.608	1509.878	2507.472	2759.32	1273.958	1474.422	1573.163	1773.773	1883.657	1626.846
34	14	unidentified	*	42.828	38.483	46.46	12.326	7.933	11.736	151.105	493.782	373.087	17.57	202.367	237.465	106.7	123.22	204.505	31.853	28.047	43.437
35	1-Hydroxy-2-propanone	C116096	C3H6O2	230.243	223.49	222.957	289.911	336.086	187.64	595.407	787.747	774.92	268.653	243.771	281.471	665.923	759.301	786.922	310.52	356.19	344.441
36	1-Penten-3-ol (E)-D	R292894	C5H10O	903.474	591.892	1673.982	898.022	1028.213	299.266	7292.057	6909.349	7697.914	281.873	4719.333	4972.738	7196.84	6632.69	6628.329	3860.302	4084.194	2675.42
37	1-Penten-3-ol (E)-M	R292894	C5H10O	654.549	558.304	760.96	971.91	995.025	663.938	1294.341	1198.09	1141.279	805.345	1417.719	1474.19	803.836	1022.78	1023.29	1396.381	1450.07	1256.54
38	15	unidentified	*	204.178	144.526	207.201	398.34	453.942	290.27	129.24	155.073	152.288	167.215	344.172	366.525	90.745	98.208	114.953	272.158	308.54	276.259
39	16	unidentified	*	650.577	727.492	682.595	179.288	180.677	132.307	903.551	1064.089	1092.167	154.064	492.336	495.156	924.977	972.808	1023.008	259.102	263.079	252.031
40	5-Methylfurfural-M	C620020	C6H6O2	159.418	201.362	188.29	546.891	549.559	435.62	275.101	282.758	287.805	540.062	421.683	424.461	159.967	152.76	197.108	666.079	669.603	650.054
41	5-Methylfurfural-D	C620020	C6H6O2	71.459	83.592	65.898	276.183	284.662	219.03	160.741	133.792	137.281	290.048	176.868	172.208	68.322	45.15	74.117	510.924	524.294	478.775
42	1-Propenyl propyl disulfide	C5905464	C6H12S2	2838.245	3268.02	2711.099	693.409	637.743	547.624	828.631	726.03	835.676	531.288	422.403	366.62	1488.039	1098.755	1256.838	1009.965	963.955	986.203
43	17	unidentified	*	28.196	31.495	39.365	8.488	5.123	9.51	43.713	49.039	64.534	9.843	11.736	9.081	65.353	80.03	106.5	10.744	9.091	7.828
44	Ethyl 2-methylpropanoate	C97621	C6H12O2	15.378	15.327	36.776	29.592	27.99	27.479	60.88	104.137	127.635	23.704	37.763	41.677	78.555	105.38	123.499	32.798	32.897	33.154
45	2-Methylbutanal	C96173	C5H10O	81.819	95.801	81.679	79.709	84.09	19.2	39.742	74.079	57.832	66.434	87.471	92.083	115.87	116.006	107.379	88.74	90.764	70.441
46	18	unidentified	*	10.531	16.726	15.53	11.178	5.653	12.666	117.643	79.909	112.219	7.978	7.924	5.342	205.711	161.372	230.002	9.649	4.45	9.916
47	19	unidentified	*	36.224	39.856	55.297	13.294	4.926	11.197	211.347	242.017	261.024	12.799	17.367	7.6	260.348	235.781	291.986	14.648	6.487	13.015
48	2-Methyl-3-methylthiofuran	C63012975	C6H8OS	240.932	223.747	272.126	85.441	87.119	134.15	331.718	338.306	303.487	76.832	65.717	64.455	355.686	325.076	370.087	120.847	125.304	149.461
49	20	unidentified	*	28.475	22.683	18.819	20.529	15.689	26.784	21.278	27.923	21.065	95.823	20.688	15.806	537.102	386.841	500.504	26.039	10.119	26.083
50	Dipropyl sulfide	C111477	C6H14S	681.967	700.571	646.936	831.388	806.211	627.339	124.92	196.071	179.846	654.498	198.085	178.641	66.012	51.729	50.536	634.616	677.324	723.47
51	Diallyl sulfide	C592881	C6H10S	1368.921	1533.367	1140.194	1424.142	1487.04	1362.983	929.773	626.562	680.981	1798.8	4448.86	4236.044	999.04	1022.888	1014.044	1885.047	1955.132	1813.185

Table S2. Differential markers in garlic samples from different origins.

No.	Var ID (Primary)	CAS#	Formula	MW	RI	Rt[sec]	Dt[RIPrel]	Comment	VIP score	*p*-value
1	1-Penten-3-ol (E)-D	R292894	C5H10O	86.1	659.9	149.793	1.3344	Dimer	2.44827	4.70×10-4
2	Diallyldisulfide	C2179579	C6H10S2	146.3	1074.4	454.021	1.6381		2.23295	1.97×10-10
3	(Z)-3-Hexen-1-ol	C928961	C6H12O	100.2	869.2	243.539	1.5102		2.06896	4.71×10-13
4	4-Ethylphenol	C123079	C8H10O	122.2	1143.2	562.46	1.2002		1.88465	2.14×10-13
5	Diallyl sulfide	C592881	C6H10S	114.2	868.2	242.92	1.1213		1.87102	2×10-3
6	1-Propenyl propyl disulfide	C5905464	C6H12S2	148.3	1099.3	493.149	1.6383		1.57428	1.64×10-9
7	Propylacetate-D	C109604	C5H10O2	102.1	715.5	168.735	1.4671	Dimer	1.3655	1.70×10-4
8	3	unidentified	*	0	1004.5	354.606	1.1606		1.35119	1.21×10-14
9	1-Propene-1-methylthio	R301790	C4H8S	88.2	724.2	172.3	1.0402		1.33622	2.30×10-2
10	3,4-Dimethylthiophene	C632155	C6H8S	112.2	885	252.866	1.1404		1.33362	2.42×10-14
11	Isoeugenol	C97541	C10H12O2	164.2	1429.8	1014.504	1.2934		1.32686	5.25×10-10
12	2-Ethylfuran	C3208160	C6H8O	96.1	708.9	166.144	1.3078		1.21905	3.00×10-5
13	4	unidentified	*	0	930.5	283.401	1.4603		1.10348	2×10-5
14	1-Penten-3-ol (E)-M	R292894	C5H10O	86.1	661.7	150.297	1.0949	Monomer	1.08732	5×10-3
15	10	unidentified	*	0	758.9	187.595	1.3497		1.0762	1×10-5
16	1	unidentified	*	0	1046.6	411.667	1.2114		1.0571	7.88×10-12