

Table S1. Detail information of samples.

No.	Name	Flavor	Ethanol Content (V/V)	Years	Origin
S1	20Nian jiaocang	Sauce flavor	53	2021	Gui zhou
S2	Mao tai wang zi jiu	Sauce flavor	53	2021	Gui zhou
S3	Sicanglaojiu	Sauce flavor	53	2021	Gui zhou
S4	Xi jiu (jun ping)	Sauce flavor	53	2021	Gui zhou
S5	Qing hualang (20)	Sauce flavor	53	2021	Si chun
S6	Guojiao (1573)	Strong flavor	52	2020	Si chun
S7	Jian nanchun (shui jing jian)	Strong flavor	52	2021	Si chun
S8	Tai wan xiaojiu	Strong flavor	52	2019	Fu jian
S9	Wu liang ye (di ba dai)	Strong flavor	52	2020	Si chun
S10	Er guotou (xiao fang ping)	Light flavor	42	2020	Bei jing
S11	Er guotou (hong xing)	Light flavor	56	2020	Bei jing
S12	Jiang xiao bai	Light flavor	52	2019	Chong qin
S13	Lao baigan (fu yang he)	Light flavor	52	2021	He bei
S14	Er guotou (niu lan shan)	Light flavor	52	2021	Bei jing
S15	Yi danliang	Light flavor	42	2021	Bei jing

Table S2 Detected DnsCl labeled amino and phenolic compounds in Baijiu.

No.	tr /min	m/z	Name	Formula	MW	Databases	CID	Level
1*	13.1	307.1474	Butan-1-Amine	C4H11N	73.0891	Baijiu	8007	level 1
2*	4.6	309.0907	2-Aminoacetic Acid	C2H5NO2	75.0320	Baijiu	750	level 1
3*	15.2	321.1636	Pentan-1-Amine	C5H13N	87.1048	MOMA	8060	level 1
4*	5.4	323.1063	Alanine	C3H7NO2	89.0477	Baijiu	239	level 1
5	6.7	323.1063	2-(Methylamino)Acetic Acid	C3H7NO2	89.0477	Baijiu	1088	level 1
6	17.6	328.0998	Phenol	C6H6O	94.0419	Baijiu	996	level 1
7	17.9	335.1795	Hexan-1-Amine	C6H15N	101.1204	Baijiu	8102	level 1
8*	6.5	337.1224	2-Aminobutanoic Acid	C4H9NO2	103.0633	Baijiu	6657	level 1
9	3.6	339.0985	Serine	C3H7NO3	105.0426	Baijiu	617	level 1
10	7.2	349.1216	Proline	C5H9NO2	115.0633	Baijiu	614	level 1
11	20.2	349.1936	Heptan-1-Amine	C7H17N	115.1361	Baijiu	8127	level 1
12*	5.9	351.1343	5-Aminopentanoic Acid	C5H11NO2	117.0790	Baijiu	138	level 1
13	4.3	353.1165	Threonine	C4H9NO3	119.0582	Baijiu	205	level 1
14	13.5	355.1482	2-Phenylethylamine	C8H11N	121.0891	Baijiu	7408	level 1
15	15.6	356.0957	4-Hydroxybenzaldehyde	C7H6O2	122.0368	Baijiu	126	level 1
16*	21.2	356.1304	4-Ethylphenol	C8H10O	122.0732	Baijiu	31242	level 1
17*	22.0	363.2108	Octan-1-Amine	C8H19N	129.1517	Baijiu	8143	level 1
18*	12.2	599.1993	Ornithine	C5H12N2O2	132.0899	Baijiu	389	level 1
19*	21.4	302.6004	Tyramine	C8H11NO	137.0841	Baijiu	5610	level 1
20	13.1	307.1156	Lysine	C6H14N2O2	146.1055	Baijiu	866	level 1
21*	15.5	386.1065	2-Vanillin	C8H8O3	152.0473	MOMA	8991	level 1
22*	18.6	620.1884	Octopamine	C8H11NO2	153.0790	Baijiu	4581	level 1
23*	13.7	398.1061	4-Hydroxycinnamic Acid	C9H8O3	164.0473	Baijiu	322	level 1
24*	13.2	400.1213	Peonol	C9H10O3	166.0630	Baijiu	11092	level 1
25*	15.8	412.1212	Coniferaldehyde	C10H10O3	178.0630	Baijiu	9984	level 1
26	17.7	324.5957	Tyrosine	C9H11NO3	181.0739	Baijiu	1153	level 1
27*	14.7	416.1168	Syringic aldehyde	C9H10O4	182.0579	Baijiu	8655	level 1
28	25.2	419.2726	Dodecan-1-Amine	C12H27N	185.2143	MOMA	13583	level 1
29*	19.5	428.1531	4-Allylsyringol	C11H14O3	194.0943	YMDB	226486	level 1
30	9.5	464.2213	Ile-Val	C11H22N2O3	230.1630	Baijiu	435949	level 1
31	11.3	385.1218	2,3-Dihydro-1H-Indole-5,6-Diol	C8H9NO2	151.0633	FDB	147311	level 2
32	11.3	412.0886	5,7-Dihydroxychromen-4-One	C9H6O4	178.0266	FDB	5281343	level 2
33	18.1	414.1376	Propyl 4-hydroxybenzoate	C10H12O3	180.0786	Baijiu	7175	level 2
34	16.0	442.0937	Fraxetin	C10H8O5	208.0372	MOMA	5273569	level 2
35	19.3	442.1329	Methyl 3-(4-Hydroxy-3-Methoxyphenyl) Prop-2-Enoate	C11H12O4	208.0736	FDB	16830	level 2
36	20.6	444.1474	5-(3,5-Dihydroxyphenyl) Pentanoic Acid	C11H14O4	210.0892	FDB	14080911	level 2
37	15.1	490.2370	4-(3-Ethenyl-3,7-Dimethylocta-1,6-Dienyl) Phenol	C18H24O	256.1827	Baijiu	500216	level 2
38	20.7	504.2044	6-(2,4-Dihydroxy-3,5-Dimethylhexyl)-4-Hydroxy-3-Methylpyran-2-One	C14H22O5	270.1467	MOMA	54738509	level 2
39	16.3	319.1476	Pent-4-En-1-Amine	C5H11N	85.0891	Baijiu	533854	level 3

40	12.1	329.0962	Pyridin-3-Ol	C5H5NO	95.0371	Baijiu	7971	level 3
41	5.4	337.1224	4-Aminobutanoic Acid	C4H9NO2	103.0633	MOMA	119	level 3
42	17.8	355.1480	2-Phenylethanamine	C8H11N	121.0891	MOMA	1001	level 3
43	10.6	365.1537	2-Amino-3-Methylpentanoic Acid	C6H13NO2	131.0946	YMDB	791	level 3
43	10.6	365.1537	2-Amino-4-Methylpentanoic Acid	C6H13NO2	131.0946	YMDB	857	level 3
44	3.8	367.0958	2-Aminobutanedioic Acid	C4H7NO4	133.0375	MOMA	424	level 3
45	19.7	369.1634	1-Phenylpropan-2-Amine	C9H13N	135.1048	FDB	3007	level 3
46	12.8	372.0902	2-Hydroxybenzoic Acid	C7H6O3	138.0317	MOMA	338	level 3
47	10.8	373.1223	5-Aminocyclohexa-1,3-Diene-1-Carboxylic Acid	C7H9NO2	139.0633	MOMA	3445	level 3
48	3.8	381.1115	2-Aminopentanedioic Acid	C5H9NO4	147.0532	MOMA	611	level 3
49	14.7	390.1012	2-Methoxybenzene-1,3,5-Triol	C7H8O4	156.0423	MOMA	4303263	level 3
50	9.3	399.1373	2-Amino-3-Phenylpropanoic Acid	C9H11NO2	165.0790	MOMA	994	level 3
51	20.1	400.1216	Ethylparaben	C9H10O3	166.0630	MOMA	8434	level 3
52	16.5	404.1164	4-(1,2-Dihydroxyethyl) Benzene-1,2-Diol	C8H10O4	170.0579	MOMA	91528	level 3
53	2.5	408.1704	Arginine	C6H14N4O2	174.1117	MOMA	232	level 3
54	15.3	410.1061	3-Amino-2-(Oxaloamino)Propanoic Acid	C5H8N2O5	176.0433	FDB	107978	level 3
55	2.6	413.1375	2-Amino-3,4,5,6-Tetrahydroxyhexanal	C6H13NO5	179.0794	MOMA	318324	level 3
56	4.6	415.1327	Beta-Tyrosine	C9H11NO3	181.0739	FDB	23395	level 3
57	10.3	416.1168	2-Hydroxy-3-(4-Hydroxyphenyl) Propanoic Acid	C9H10O4	182.0579	MOMA	9378	level 3
58	13.1	421.1797	8-Amino-7-Oxononanoic Acid	C9H17NO3	187.1208	YMDB	173	level 3
59	12.8	430.1328	Dihydroferulic Acid	C10H12O4	196.0736	MOMA	14340	level 3
60	15.1	444.1477	1-(2-Hydroxy-4,6-Dimethoxy-3-Methylphenyl) Ethanone	C11H14O4	210.0892	FDB	326186	level 3
60	15.1	444.1477	4-(3-Hydroxyprop-1-Enyl)-2,6-Dimethoxyphenol	C11H14O4	210.0892	FDB	439703	level 3
61	11.6	458.1268	3-(4-Hydroxy-3,5-Dimethoxyphenyl) Prop-2-Enoic Acid	C12H14O4	222.0892	MOMA	10743	level 3
62	11.9	458.1271	O-Methylcurvulinic acid	C11H12O5	224.0685	Baijiu	16745395	level 3
63	15.1	460.1427	5-(3,4-Dihydroxyphenyl)-4-Hydroxypentanoic Acid	C11H14O5	226.0841	FDB	52920332	level 3
63	15.1	460.1427	3-(4-Hydroxy-3,5-Dimethoxyphenyl) Propanoic Acid	C11H14O5	226.0841	FDB	84681	level 3
63	15.1	460.1427	5-(3,5-Dihydroxyphenyl)-4-Hydroxypentanoic Acid	C11H14O5	226.0841	FDB	52920333	level 3
64	13.5	464.2216	2-[(2-Amino-3-Methylbutanoyl) Amino]-3-Methylpentanoic Acid	C11H22N2O3	230.1630	FDB	5246013	level 3
65	21.8	468.1476	2-[(2-Amino-3-Hydroxypropanoyl) Amino] Pentanedioic Acid	C8H14N2O6	234.0852	FDB	3613616	level 3
65	21.8	468.1476	4-Amino-5-[(1-Carboxy-2-Hydroxyethyl) Amino]-5-Oxopentanoic Acid	C8H14N2O6	234.0852	FDB	428748	level 3
65	21.8	468.1476	2-Amino-5-[(1-Carboxy-2-Hydroxyethyl) Amino]-5-Oxopentanoic Acid	C8H14N2O6	234.0852	FDB	5317735	level 3
65	21.8	468.1476	2-[(2-Amino-3-Hydroxybutanoyl) Amino] Butanedioic Acid	C8H14N2O6	234.0852	FDB	3280446	level 3
66	13.6	470.1270	2-(7-Hydroxy-2-Methyl-4-Oxo-2,3-Dihydrochromen-5-Yl) Acetic Acid	C12H12O5	236.0685	FDB	591742	level 3
67	18.1	472.1425	2-(2-Acetyl-3,5-Dihydroxy-4,6-Dimethylphenyl) Acetic Acid	C12H14O5	238.0841	MOMA	44715172	level 3
68	17.5	474.1581	Propan-2-Yl 3-(3,4-Dihydroxyphenyl)-2-Hydroxypropanoate	C12H16O5	240.0998	FDB	44234503	level 3
69	14.0	492.1511	3,4,4-Trihydroxyflavan	C15H14O4	258.0892	FDB	85979126	level 3
70	17.0	500.1373	6,8-Dihydroxy-3,4,5-Trimethyl-1-Oxo-3,4-Dihydroisochromene-7-Carboxylic Acid	C13H14O6	266.0790	MOMA	15558919	level 3
71	21.8	508.1433	2-(3,4-Dihydroxyphenyl)-3,4-Dihydro-2H-Chromene-3,7-Diol	C15H14O5	274.0841	FDB	3984814	level 3
72	16.5	524.2216	8-Hydroxy-5-[1-Hydroxy-2-(Propan-2-Ylamino) Butyl]-1H-Quinolin-2-One	C16H22N2O3	290.1630	Baijiu	4916	level 3
73	15.7	530.1853	Phenylalanylmethionine	C15H20O6	296.1260	FDB	139852	level 3
74	21.7	534.1808	2-(Hydroxymethyl)-6-[2-(4-Hydroxyphenyl) Ethoxy] Oxane-3,4,5-Triol	C14H20O7	300.1209	FDB	4961358	level 3

75	18.1	321.1280	4-Aminobutanal	C4H9NO	87.0684	YMDB	118	level 4
76	14.9	321.1634	Pentan-2-Amine	C5H13N	87.1048	Baijiu	12246	level 4
76	14.9	321.1634	2-Methylbutan-1-Amine	C5H13N	87.1048	Baijiu	7283	level 4
77	15.1	333.1637	Cyclohexanamine	C6H13N	99.1048	FDB	7965	level 4
78	11.3	343.1112	4-Aminophenol	C6H7NO	109.0528	MOMA	403	level 4
79	13.0	343.1117	3-Aminophenol	C6H7NO	109.0528	MOMA	11568	level 4
80	13.2	343.1120	2-Aminophenol	C6H7NO	109.0528	MOMA	5801	level 4
81	10.4	351.1114	2-(Diaminomethylideneamino)Acetic Acid	C3H7N3O2	117.0538	FDB	763	level 4
82	10.8	355.1118	4-Aminobenzaldehyde	C7H7NO	121.0528	FDB	11158	level 4
83	18.0	356.1319	2,4-Dimethylphenol	C8H10O	122.0732	Baijiu	7771	level 4
84	14.1	357.1269	2-Amino-4-Methylphenol	C7H9NO	123.0684	MOMA	7264	level 4
85	12.8	357.1273	2-Methoxyaniline	C7H9NO	123.0684	MOMA	7000	level 4
85	12.8	357.1273	p-Anisidine	C7H9NO	123.0684	MOMA	7732	level 4
86	11.2	361.1589	8-Azabicyclo[3.2.1]Octan-3-Ol	C7H13NO	127.0997	MOMA	68147	level 4
87	16.9	369.1276	2-Amino-1-Phenylethanone	C8H9NO	135.0684	FDB	11952	level 4
88	15.9	370.1108	3-Hydroxy-2-Methylbenzaldehyde	C8H8O2	136.0524	Baijiu	585876	level 4
89	17.0	370.1114	2-Hydroxy-6-Methylbenzaldehyde	C8H8O2	136.0524	Baijiu	585174	level 4
90	17.9	373.0859	4-(Aminomethyl) Benzene-1,2-Diol	C6H5NO3	139.0269	Baijiu	91623	level 4
91	15.8	373.1218	4-Nitrophenol	C7H9NO2	139.0633	MOMA	980	level 4
92	21.3	377.1535	8-Azabicyclo[3.2.1]Octane-3,6-Diol	C7H13NO2	143.0946	Baijiu	22297531	level 4
93	13.3	377.1535	4-Amino-5-Methylhex-2-Enoic Acid	C7H13NO2	143.0946	FDB	567662	level 4
94	12.0	379.1692	3-Amino-5-Methylhexanoic Acid	C7H15NO2	145.1103	MOMA	2733735	level 4
95	13.9	379.1692	3-Amino-4-Methylhexanoic Acid	C7H15NO2	145.1103	MOMA	2764414	level 4
96	14.2	379.1693	Methyl 2-Amino-4-Methylpentanoate	C7H15NO2	145.1103	MOMA	410817	level 4
97	13.6	384.0906	4-Hydroxy-3H-2-Benzofuran-1-One	C8H6O3	150.0317	FDB	12662077	level 4
98	18.3	385.1222	4-(2-Aminoethyl) Cyclohexa-3,5-Diene-1,2-Dione	C8H9NO2	151.0633	FDB	162602	level 4
98	18.3	385.1222	4-(Methylamino)Benzoic Acid	C8H9NO2	151.0633	FDB	66345	level 4
98	18.3	385.1222	N-(2-Hydroxyphenyl) Acetamide	C8H9NO2	151.0633	FDB	11972	level 4
98	18.3	385.1222	4-(2-Hydroxyiminoethyl) Phenol	C8H9NO2	151.0633	FDB	152653	level 4
99	16.3	393.1851	8-Aminooctanoic Acid	C8H17NO2	159.1259	MOMA	66085	level 4
99	16.3	393.1851	2-Aminooctanoic Acid	C8H17NO2	159.1259	MOMA	69522	level 4
100	16.1	396.0916	7-Hydroxychromen-2-One	C9H6O3	162.0317	FDB	5281426	level 4
101	15.0	398.1034	3-(2-Hydroxyphenyl) Prop-2-Enoic Acid	C9H8O3	164.0473	FDB	11968	level 4
102	14.7	398.1044	3-(3-Hydroxyphenyl) Prop-2-Enoic Acid	C9H8O3	164.0473	FDB	11496	level 4
103	17.0	398.1062	7-Hydroxy-2,3-Dihydrochromen-4-One	C9H8O3	164.0473	MOMA	10855817	level 4
104	17.9	400.1207	2-(4-Hydroxyphenyl) Propanoic Acid	C9H10O3	166.0630	MOMA	102526	level 4
105	19.5	400.1217	4-(3-Hydroxyprop-1-enyl) benzene-1,2-diol	C9H10O3	166.0630	MOMA	361171	level 4
106	12.0	401.1513	4-[1-Hydroxy-2-(Methylamino) Ethyl] Phenol	C9H13NO2	167.0946	MOMA	7172	level 4
107	15.0	401.1538	Deoxyepinephrine	C9H13NO2	167.0946	Baijiu	4382	level 4
108	11.6	404.1158	Dihydrofumigatin	C8H10O4	170.0579	FDB	25244596	level 4
109	14.8	412.0829	7,8-Dihydroxychromen-2-One	C9H6O4	178.0266	MOMA	5280569	level 4
110	16.4	412.1192	Methyl 3-(4-Hydroxyphenyl) Prop-2-Enoate	C10H10O3	178.0630	MOMA	92203	level 4

111	16.1	412.1199	3-(4-Hydroxy-2-Methoxyphenyl)-2-Propenal	C10H10O3	178.0630	FDB	19082	level 4
112	16.8	415.1690	3-[2-(Ethylamino)-1-Hydroxyethyl] Phenol	C10H15NO2	181.1103	MOMA	3306	level 4
112	16.3	415.1665	2-(3,4-Dimethoxyphenyl) Ethanamine	C10H15NO2	181.1103	MOMA	8421	level 4
112	16.3	415.1665	2-(3,5-Dimethoxyphenyl) Ethanamine	C10H15NO2	181.1103	MOMA	137857	level 4
112	16.3	415.1665	2-(2,5-Dimethoxyphenyl) Ethanamine	C10H15NO2	181.1103	MOMA	76632	level 4
114	14.2	416.1515	2-(2-Hydroxypropyl)-5-Methoxyphenol	C10H14O3	182.0943	FDB	10655013	level 4
114	14.2	416.1515	4-(3-Hydroxypropyl)-2-Methoxyphenol	C10H14O3	182.0943	FDB	16822	level 4
114	14.2	416.1515	2-Ethoxy-4-(Methoxymethyl)Phenol	C10H14O3	182.0943	FDB	6453284	level 4
114	14.2	416.1515	4-Ethyl-2,6-Dimethoxyphenol	C10H14O3	182.0943	FDB	61712	level 4
115	14.8	418.1148	3,5-Dimethyl-4-Methylsulfinylphenol	C9H12O2S	184.0558	MOMA	3029900	level 4
116	12.4	418.1320	1-(4-Hydroxyphenyl) Propane-1,2,3-Triol	C9H12O4	184.0736	FDB	11095273	level 4
117	12.4	418.1320	1-(3-Hydroxy-4-Methoxyphenyl) Ethane-1,2-Diol	C9H12O4	184.0736	FDB	170451	level 4
117	13.1	418.1325	1-(4-Hydroxy-3-Methoxyphenyl) Ethane-1,2-Diol	C9H12O4	184.0736	MOMA	10805	level 4
118	14.6	418.1326	Antiarol	C9H12O4	184.0736	MOMA	69505	level 4
119	13.1	422.1264	2-Pyridin-1-ium-1-ylbenzene-1,4-Diol	C11H10NO2+	188.0712	FDB	411955	level 4
120	18.1	422.1413	Makaluvamine I	C10H10N3O+	188.0818	MOMA	135600871	level 4
121	16.4	424.1216	5-(4-Hydroxyphenyl) Penta-2,4-Dienoic Acid	C11H10O3	190.0630	FDB	589488	level 4
121	16.4	424.1216	5-Hydroxy-2-Methyl-2,3-Dihydronaphthalene-1,4-Dione	C11H10O3	190.0630	FDB	14412241	level 4
121	16.4	424.1216	7-Hydroxy-2,5-Dimethylchromen-4-One	C11H10O3	190.0630	FDB	5316891	level 4
122	18.5	426.1339	Serylserine	C6H12N2O5	192.0746	FDB	138784	level 4
123	18.2	426.1347	5-[(4-Hydroxyphenyl) Methyl] Oxolan-2-One	C11H12O3	192.0786	FDB	11550142	level 4
124	19.2	426.1367	Dehydrozingerone	C11H12O3	192.0786	FDB	59039607	level 4
125	20.4	426.1374	p-Coumaric acid ethyl ester	C11H12O3	192.0786	FDB	676946	level 4
126	15.6	427.1688	Ethyl 2-(Ethylamino)Benzoate	C11H15NO2	193.1103	FDB	61980	level 4
126	15.6	427.1688	Butyl 2-Aminobenzoate	C11H15NO2	193.1103	FDB	24433	level 4
126	15.6	427.1688	2-Methylpropyl 2-Aminobenzoate	C11H15NO2	193.1103	FDB	24515	level 4
126	15.6	427.1688	1,2-Dimethyl-3,4-Dihydro-1H-Isoquinoline-6,7-Diol	C11H15NO2	193.1103	FDB	420804	level 4
126	15.6	427.1688	1,2-Dimethyl-3,4-Dihydro-1H-Isoquinoline-5,6-Diol	C11H15NO2	193.1103	FDB	15859919	level 4
127	11.8	430.1320	5-Hydroxy-coniferyl-alcohol	C10H12O4	196.0736	FDB	5282095	level 4
128	19.5	430.1321	2-Methyl-1-(2,4,6-Trihydroxyphenyl) Propan-1-One	C10H12O4	196.0736	FDB	5326317	level 4
129	20.0	432.1483	3-(4-Hydroxy-3-Methoxyphenyl) Propane-1,2-Diol	C10H14O4	198.0892	FDB	161566	level 4
130	21.6	432.1844	3-Methylimidazo[4,5-F] Quinolin-2-Amine	C11H10N4	198.0905	MOMA	53462	level 4
131	21.7	435.2310	11-Aminoundecanoic Acid	C11H23NO2	201.1729	MOMA	17083	level 4
132	18.3	436.1433	1,6-Dimethyl-1H-1,3,4-Triaza-7-Oxa-S-Indacene-2-Amine	C10H10N4O	202.0855	FDB	71313206	level 4
133	20.1	440.1508	4-Hydroxy-3-(3-Methylbut-2-Enyl) Benzoic Acid	C12H14O3	206.0943	MOMA	443852	level 4
134	15.2	442.1311	3-(4-Hydroxy-3,5-Dimethoxyphenyl) Prop-2-Enal	C11H12O4	208.0736	MOMA	119216	level 4
135	18.4	442.1321	3-Methyl-6-Hydroxy-8-Methoxy-3,4-Dihydroisocoumarin	C11H12O4	208.0736	MOMA	16757192	level 4
136	21.0	442.1322	8-Hydroxy-6-Methoxy-3-Methylisochroman-1-One	C11H12O4	208.0736	FDB	93040	level 4
137	14.3	444.1476	5-(3,4-Dihydroxyphenyl)-valeric acid	C11H14O4	210.0892	FDB	49831816	level 4
138	12.0	445.1796	Metaproterenol	C11H17NO3	211.1208	Baijiu	4086	level 4
139	16.4	446.1029	2-Hydroxyxanthen-9-One	C13H8O3	212.0473	FDB	74708	level 4
139	16.4	446.1029	3-Hydroxybenzo[C]Chromen-6-One	C13H8O3	212.0473	FDB	5380406	level 4

139	16.4	446.1029	4-Hydroxyxanthen-9-One	C13H8O3	212.0473	FDB	611428	level 4
140	15.6	449.1508	N-(4-Hydroxy-3-Methylnaphthalen-1-Yl) Acetamide	C13H13NO2	215.0946	FDB	124103	level 4
141	17.9	451.1612	Alanyl-Gamma-Glutamate	C8H15N3O4	217.1063	FDB	131750731	level 4
141	17.9	451.1612	2-[(2,5-Diamino-5-Oxopentanoyl) Amino] Propanoic Acid	C8H15N3O4	217.1063	FDB	20073769	level 4
142	18.6	454.1320	5-Hydroxy-7-Methoxy-2,6-Dimethylchromen-4-One	C12H12O4	220.0736	FDB	3083581	level 4
142	18.6	454.1320	5-Hydroxy-7-Methoxy-2,8-Dimethylchromen-4-One	C12H12O4	220.0736	FDB	12310980	level 4
142	18.6	454.1320	6-(3,4-Dihydroxyphenyl)-4-Hydroxyhexa-3,5-Dien-2-One	C12H12O4	220.0736	FDB	53395354	level 4
143	14.1	456.1108	2-[3-(4-Hydroxyphenyl) Prop-2-Enoyloxy] Acetic Acid	C11H10O5	222.0528	FDB	85826693	level 4
143	14.1	456.1108	7-Hydroxy-6,8-Dimethoxychromen-2-One	C11H10O5	222.0528	FDB	5318565	level 4
143	14.1	456.1108	6-Hydroxy-5,7-Dimethoxychromen-2-One	C11H10O5	222.0528	FDB	3047739	level 4
144	16.7	456.1469	3-(4-Hydroxy-3-Methoxyphenyl) Prop-2-Enyl Acetate	C12H14O4	222.0892	FDB	25200581	level 4
145	21.8	456.1479	Sclerotinin C	C12H14O4	222.0892	MOMA	102595352	level 4
146	20.6	456.1481	5-[(4-Hydroxy-3-Methoxyphenyl) Methyl] Oxolan-2-One	C12H14O4	222.0892	FDB	3028410	level 4
147	16.0	466.0982	9-Hydroxy-4-Methoxyfuro[3,2-G] Chromen-7-One	C12H8O5	232.0372	FDB	3083726	level 4
148	12.7	472.1428	10-Norparvulenone	C12H14O5	238.0841	MOMA	9991774	level 4
148	12.7	472.1428	Ethyl 2-(2-Acetyl-3,5-Dihydroxyphenyl) Acetate	C12H14O5	238.0841	MOMA	177045	level 4
149	13.1	478.1361	4-[2-(3,5-Dihydroxyphenyl) Ethenyl] Benzene-1,2-Diol	C14H12O4	244.0736	MOMA	4813	level 4
150	14.1	478.2369	2-[(2-Amino-4-Methylpentanoyl) Amino]-3-Methylpentanoic Acid	C12H24N2O3	244.1787	FDB	435718	level 4
150	14.1	478.2369	2-[(2-Amino-3-Methylpentanoyl) Amino]-4-Methylpentanoic Acid	C12H24N2O3	244.1787	FDB	13817313	level 4
150	14.1	478.2369	2-[(2-Amino-3-Methylpentanoyl) Amino]-3-Methylpentanoic Acid	C12H24N2O3	244.1787	FDB	13879965	level 4
150	14.1	478.2369	2-[(2-Amino-4-Methylpentanoyl) Amino]-4-Methylpentanoic Acid	C12H24N2O3	244.1787	FDB	94244	level 4
151	17.6	486.1583	8-Methyl-3,4,6,10B-Tetrahydro-2H-Pyrano[3,2-C] Isochromene-4A,7,9-Triol	C13H16O5	252.0998	MOMA	75368714	level 4
152	14.1	486.1589	7-Hydroxy-8-(2-Hydroxyethyl)-5-Methoxy-2-Methyl-2,3-Dihydrochromen-4-One	C13H16O5	252.0998	MOMA	15674945	level 4
153	17.6	508.1400	2-(4-Hydroxyphenyl)-3,4-Dihydro-2H-Chromene-3,5,7-Triol	C15H14O5	274.0841	MOMA	282014	level 4
154	14.5	514.1506	Methionylmethionine	C10H20N2O3S2	280.0915	FDB	104294	level 4
155	17.6	514.1887	2-Amino-3-(1H-Imidazol-5-Yl)-N-Naphthalen-2-Ylpropanamide	C16H16N4O	280.1324	MOMA	110993	level 4
156	20.8	518.2208	4-[2-[4-(Hydroxymethyl)-7-Methyl-6,7-Dihydro-5H-Cyclopenta[C]Pyridin-2-Ium-2-Yl] Ethyl] Phenol	C18H22NO2+	284.1651	FDB	5315162	level 4
157	13.8	520.1465	3-Methoxy-6,11A-Dihydro- [1] Benzofuro[3,2-C] Chromene-6A,9-Diol	C16H14O5	286.0841	FDB	44257486	level 4
157	13.8	520.1465	9-Methoxy-6,11A-Dihydro- [1] Benzofuro[3,2-C] Chromene-3,6A-Diol	C16H14O5	286.0841	FDB	44257485	level 4
157	13.8	520.1465	2,7-Dihydroxy-3-(4-Methoxyphenyl)-2,3-Dihydrochromen-4-One	C16H14O5	286.0841	FDB	9860663	level 4
158	18.6	522.1559	2-(4-Methoxyphenyl)-1-(2,4,6-Trihydroxyphenyl) Propan-1-One	C16H16O5	288.0998	FDB	10779696	level 4
158	18.6	522.1559	1-(2,4-Dihydroxy-5-Methoxyphenyl)-2-(4-Hydroxyphenyl) Propan-1-One	C16H16O5	288.0998	FDB	71367568	level 4
158	18.6	522.1559	5,8-Dihydroxy-2-(1-Hydroxy-4-Methylpent-3-Enyl) Naphthalene-1,4-Dione	C16H16O5	288.0998	FDB	5208	level 4
159	13.3	534.2275	2-Hydroxy-3-Methoxy-13-Methyl-7,8,9,11,12,14,15,16-Octahydro-6H-Cyclopenta[A]Phenanthren-17-One	C19H24O3	300.1725	FDB	627213	level 4
159	13.3	534.2275	Sageone	C19H24O3	300.1725	FDB	6481824	level 4
160	18.6	538.1292	4-(3,4-Dihydroxyphenyl)-2-Hydroxyphenalen-1-One	C19H12O4	304.0736	FDB	10892036	level 4
161	18.6	538.1292	2,3-Dihydroxy-9-(4-Hydroxyphenyl) Phenalen-1-One	C19H12O4	304.0736	FDB	10733280	level 4
162	22.9	541.2733	N-[(4-Hydroxy-3-Methoxyphenyl) Methyl]-8-Methylnonanamide	C18H29NO3	307.2147	MOMA	107982	level 4
163	22.3	564.2031	Fragransol B	C19H22O5	330.1467	FDB	14015413	level 4
163	22.3	564.2031	5-(3,7-Dimethyl-5-Oxooccta-2,6-Dienyl)-4-Hydroxy-6-Methoxy-3H-2-Benzofuran-1-One	C19H22O5	330.1467	FDB	73099018	level 4
164	20.6	642.2186	Garcimangosone B	C24H24O6	408.1573	FDB	11143989	level 4
164	20.6	642.2186	Mammea A/Ac Cyclo F	C24H24O6	408.1573	FDB	5319254	level 4

164	20.6	642.2186	Mammea A/Ad Cyclof	C24H24O6	408.1573	FDB	44257538	level 4
165	7.1	699.2307	2-(4-Hydroxy-3,5-Dimethoxyphenyl)-3-(4-Hydroxy-3-Methoxyphenyl)-N-[2-(4-Hydroxyphenyl) Ethyl] Prop-2-Enamide	C26H27NO7	465.1788	FDB	197474	level 4
166	7.1	721.2134	Malvidin 3-Alpha-L-Galactoside	C25H27O10	487.1604	FDB	157010023	level 4
167	20.1	277.1010		C2H5N	43.0422			level 5
168	13.7	303.0802		C3H3NO	69.0215			level 5
169	7.2	303.0901		C2H3N3	69.0327			level 5
170	14.8	303.1157		C4H7N	69.0578			level 5
171	12.9	305.0956		C3H5NO	71.0371			level 5
172	8.0	306.0893		C2H4N2O	72.0324			level 5
173	8.9	319.0847		C2H3N3O	85.0276			level 5
174	12.7	320.0952		C2H4N3O	86.0354			level 5
175	7.7	321.1005		C2H5N3O	87.0433			level 5
176	10.0	331.0844		C3H3N3O	97.0276			level 5
177	16.5	333.1269		C3H7N4	99.0671			level 5
177	16.5	333.1269		C5H9NO	99.0684			level 5
178	10.3	347.1172		C4H7N3O	113.0589			level 5
179	18.5	347.1429		C6H11NO	113.0841			level 5
180	12.2	348.0916		C8H4N	114.0344			level 5
181	11.1	356.0624		C9N	122.0031			level 5
182	23.9	356.1060		C6H6N2O	122.0480			level 5
183	16.4	360.1606		C6H12N3	126.1031			level 5
184	21.9	361.0973		C4H5N3O2	127.0382			level 5
185	13.7	362.1066		C9H6N	128.0500			level 5
186	10.7	368.0987		C3H8N3OS	134.0388			level 5
187	12.2	370.0732		C5H2N3O2	136.0147			level 5
188	8.4	371.1175		C6H7N3O	137.0589			level 5
189	15.0	376.1216		C5H8N3O2	142.0616			level 5
190	15.2	376.1216		C5H8N3O2	142.0616			level 5
191	17.5	381.1277		C4H11N4S	147.0704			level 5
191	17.5	381.1277		C9H9NO	147.0684			level 5
192	12.9	384.0881		C6H4N3O2	150.0303			level 5
193	16.1	390.1373		C6H10N3O2	156.0773			level 5
194	17.8	390.1377		C11H10N	156.0813			level 5
195	14.6	391.1692		C8H15NO2	157.1103			level 5
196	10.8	392.1158		C8H6N4	158.0592			level 5
197	12.3	394.0966		C7H4N4O	160.0385			level 5
197	12.3	394.0966		C9H6NO2	160.0399			level 5
198	18.4	394.1322		C8H8N4	160.0749			level 5
199	10.4	396.0869		C7H4N3O2	162.0303			level 5
200	10.6	396.1118		C7H6N4O	162.0541			level 5
201	10.4	402.0767		C9H2N3O	168.0198			level 5

202	13.9	404.0623	C5H4N3O2S	170.0024	level 5
202	13.9	404.0623	C13N	170.0031	level 5
203	13.0	404.0991	C6H8N3OS	170.0388	level 5
204	14.1	406.0964	C8H4N4O	172.0385	level 5
204	14.1	406.0964	C10H6NO2	172.0399	level 5
205	16.5	408.1135	C8H6N4O	174.0541	level 5
205	16.5	408.1135	C10H8NO2	174.0555	level 5
206	20.1	418.1690	C13H14N	184.1126	level 5
207	10.7	420.0942	C11H8NS	186.0377	level 5
207	10.7	420.0942	C14H4N	186.0344	level 5
208	11.5	420.1111	C9H6N4O	186.0541	level 5
209	13.5	420.1114	C9H6N4O	186.0541	level 5
210	16.0	420.1118	C9H6N4O	186.0541	level 5
210	16.0	420.1118	C11H8NO2	186.0555	level 5
211	13.0	426.0811	C8H6N3OS	192.0231	level 5
212	16.4	434.1264	C10H8N4O	200.0698	level 5
213	14.4	434.1267	C10H8N4O	200.0698	level 5
214	12.1	434.1270	C10H8N4O	200.0698	level 5
215	22.6	446.2003	C10H18N3O2	212.1399	level 5
215	22.6	446.2003	C15H18N	212.1439	level 5
216	18.1	448.0881	C10H6N4S	214.0313	level 5
216	18.1	448.0881	C13H2N4	214.0279	level 5
217	11.1	448.0891	C10H6N4S	214.0313	level 5
217	11.1	448.0891	C12H8NOS	214.0327	level 5
218	16.8	448.1418	C11H10N4O	214.0854	level 5
219	15.0	448.1431	C11H10N4O	214.0854	level 5
219	15.0	448.1431	C13H12NO2	214.0868	level 5
220	10.6	451.1525	C13H15NS	217.0925	level 5
221	22.1	451.1905	C13H17N2O	217.1341	level 5
222	19.4	456.0573	C11H2N4S	222.0000	level 5
222	19.4	456.0573	C16NO	221.9980	level 5
223	16.0	458.0643	C12H4N2OS	224.0044	level 5
224	11.6	459.1302	C10H13N2O2S	225.0698	level 5
225	19.3	462.1219	C11H8N4O2	228.0647	level 5
226	16.5	462.1582	C12H12N4O	228.1011	level 5
227	20.8	462.1585	C12H12N4O	228.1011	level 5
227	20.8	462.1585	C14H14NO2	228.1025	level 5
228	18.8	462.2305	C11H22N3O2	228.1712	level 5
229	13.8	464.0810	C13H2N4O	230.0228	level 5
229	13.8	464.0810	C15H4NO2	230.0242	level 5
230	19.3	475.1539	C14H13N2O2	241.0977	level 5
231	12.8	476.1742	C13H14N4O	242.1167	level 5

231	12.8	476.1742	C15H16NO2	242.1181	level 5
232	21.9	476.2100	C14H18N4	242.1531	level 5
233	14.5	476.2222	C15H20N3	242.1657	level 5
234	17.6	478.1564	C9H16N4O2S	244.0994	level 5
234	17.6	478.1564	C12H12N4O2	244.0960	level 5
235	14.8	480.1681	C12H14N4O2	246.1117	level 5
236	10.4	486.0662	C15N4O	252.0072	level 5
236	10.4	486.0662	C17H2NO2	252.0086	level 5
237	18.0	490.1895	C14H16N4O	256.1324	level 5
238	14.1	490.1897	C14H16N4O	256.1324	level 5
238	14.1	490.1897	C16H18NO2	256.1338	level 5
239	14.5	492.1689	C13H14N4O2	258.1117	level 5
240	16.0	492.2532	C16H24N3	258.1970	level 5
241	21.8	502.1894	C15H16N4O	268.1324	level 5
242	15.8	504.1681	C14H14N4O2	270.1117	level 5
243	23.5	504.3259	C16H34N2O	270.2671	level 5
244	10.1	508.1250	C13H12N3O2S	274.0650	level 5
244	10.1	508.1250	C18H12NS	274.0690	level 5
245	17.8	511.1507	C18H15NS	277.0925	level 5
246	20.0	514.1845	C14H20N2O2S	280.1245	level 5
247	23.6	520.2365	C16H22N4O	286.1793	level 5
247	23.6	520.2365	C18H24NO2	286.1807	level 5
248	23.9	528.2050	C17H18N4O	294.1480	level 5
249	21.6	528.2054	C17H18N4O	294.1480	level 5
249	21.6	528.2054	C19H20NO2	294.1494	level 5
250	19.4	535.2458	C19H27NS	301.1864	level 5
251	18.5	542.1816	C18H18N3S	308.1221	level 5
252	21.8	546.2157	C17H20N4O2	312.1586	level 5
253	22.5	546.2519	C18H24N4O	312.1950	level 5
254	18.7	548.1931	C17H20N3OS	314.1327	level 5
255	25.5	569.3048	C15H35N4O2S	335.2481	level 5
255	25.5	569.3048	C18H31N4O2	335.2447	level 5
256	25.5	591.2863	C20H29N4O2	357.2290	level 5
257	21.2	594.3359	C22H36N2O2	360.2777	level 5
258	22.3	596.3505	C22H38N2O2	362.2933	level 5
259	20.7	612.3439	C23H40NOS	378.2831	level 5
260	19.0	619.3527	C23H37N4O	385.2967	level 5
261	12.8	742.3560	C30H42N3O2S	508.2998	level 5
261	12.8	742.3560	C33H38N3O2	508.2964	level 5
262	10.6	745.4056	C30H47N4OS	511.3470	level 5
262	10.6	745.4056	C32H49NO2S	511.3484	level 5
262	10.6	745.4056	C35H45NO2	511.3450	level 5

263	18.2	812.4318	C38H48N3O2	578.3746	level 5
263	18.2	812.4318	C39H50N2S	578.3695	level 5
264	15.7	821.2300	C43H25NS	587.1708	level 5
265	20.1	826.4516	C36H54N3O2S	592.3937	level 5
265	20.1	826.4516	C39H50N3O2	592.3903	level 5
266	17.6	894.4433	C42H52N4OS	660.3862	level 5
266	17.6	894.4433	C44H54NO2S	660.3875	level 5
267	18.4	908.4565	C43H54N4OS	674.4018	level 5
267	18.4	908.4565	C46H50N4O	674.3984	level 5

a) * represents the compounds are related to flavor or biological activity, b) WM represents molecular weight, c) CID represents Compound CID from Pubchem, d) Baijiu represents the compounds reported from Baijiu database, e) YMDB represents the compounds in The Yeast Metabolome Database, f) FDB represents the compounds in The Food Database, g) MoNA represents the compounds in MassBank of North America.

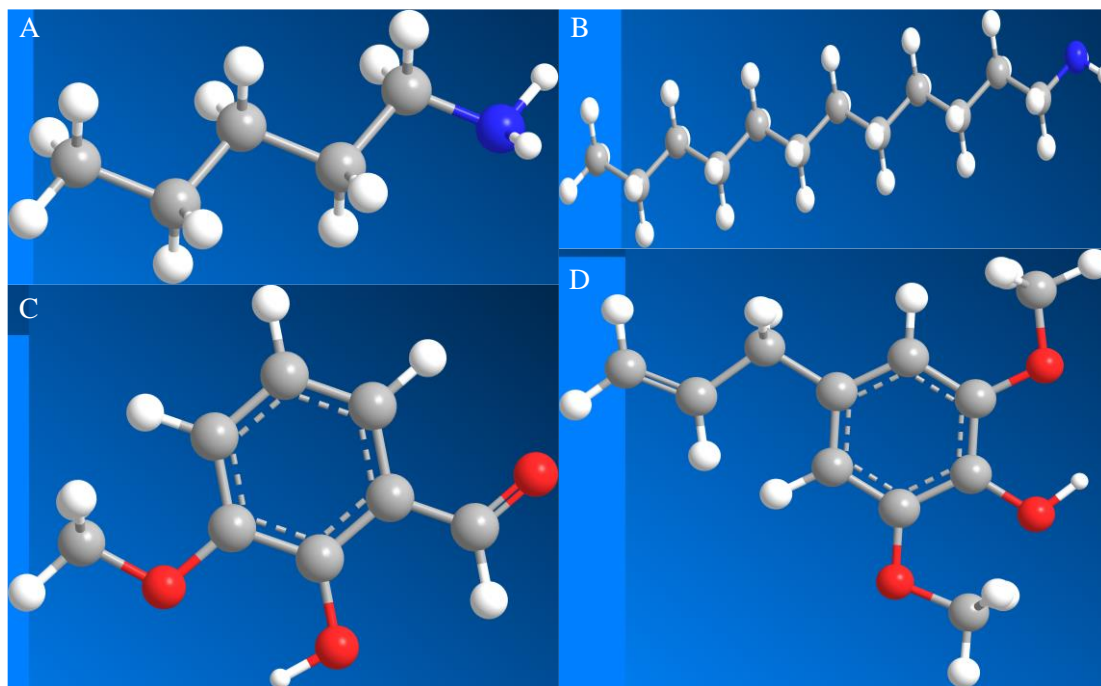


Figure S1. The 3D structure of four newly identified compounds. The A, B, C and D are pentan-1-amine, dodecan-1-amine, 2-vanillin and 4-allylsyringol, respectively.