

Comprehensive Real-Time Analysis of the Yeast Volatilome

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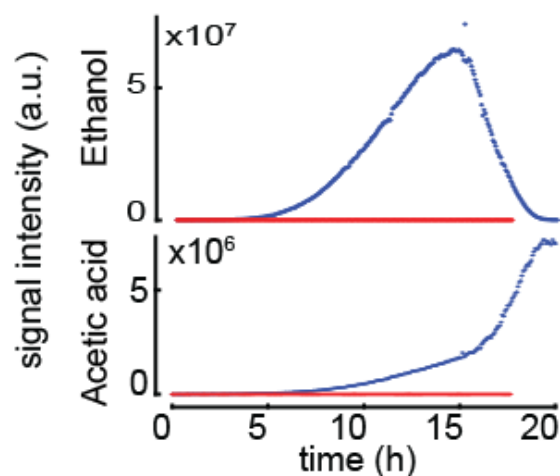


Figure S1. Signal intensity of ethanol and acetic acid after $^{13}\text{C}_6$ -glucose injection in a solution containing yeast (same as Figure 1b; blue) and a negative control (red) under exactly the same conditions, but without yeast. As expected, ethanol and acetic acid production can be attributed to yeast growth.

Supporting Information

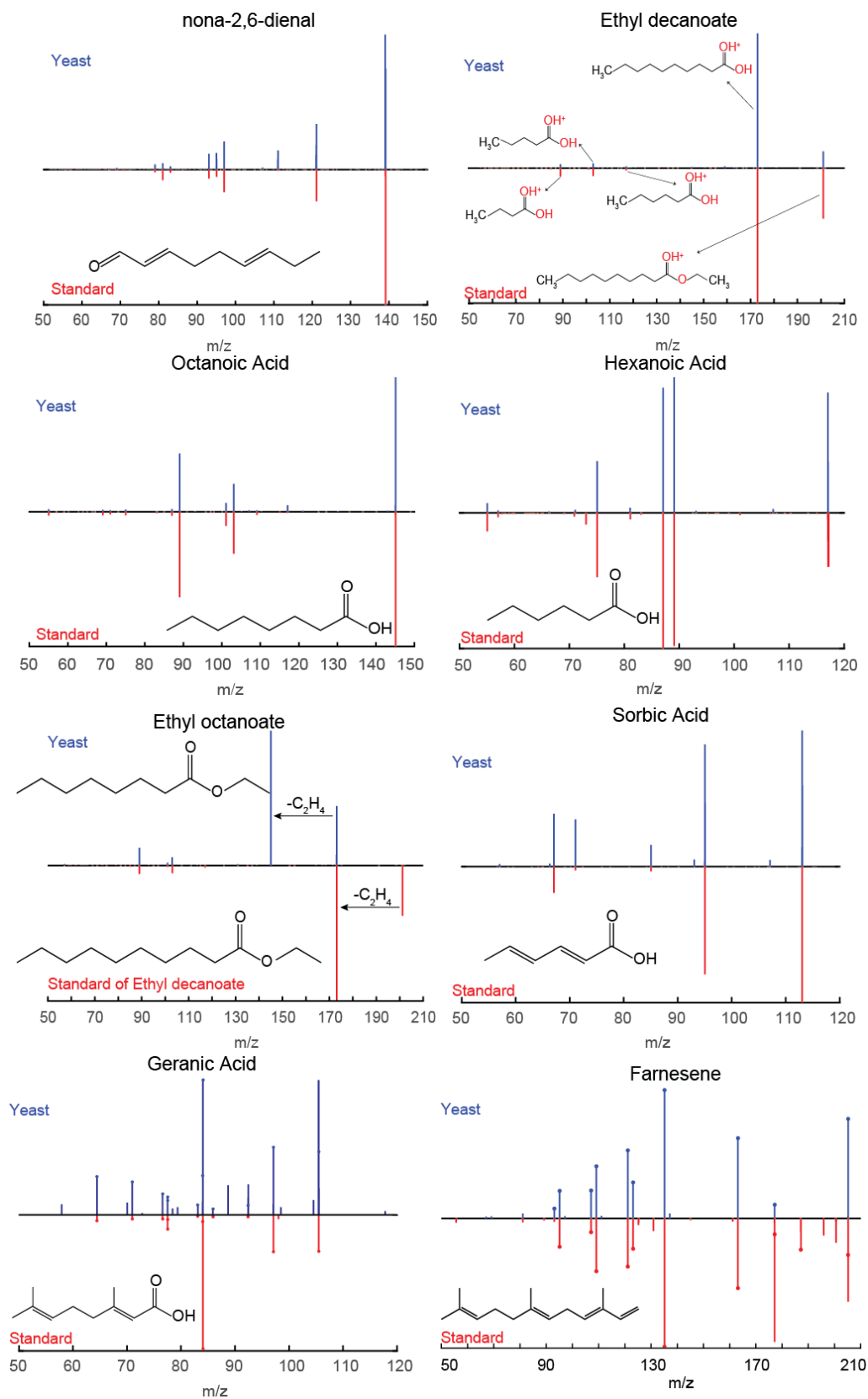


Figure S2. Head-to-tail MS/MS mass spectra of selected yeast metabolites (top) and standards (bottom).

Supporting Information

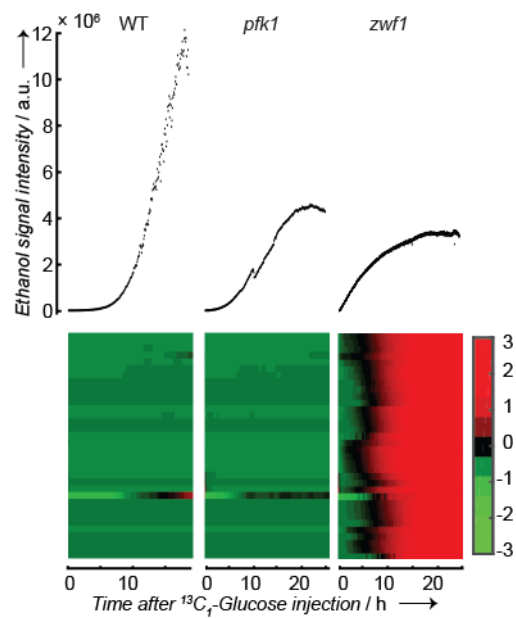


Figure S3. Replicated experiment injecting $^{13}\text{C}_1$ -glucose to the cultivations of the three yeast strains WT, *pfk1*, *zwf1* provided a similar global picture as that shown in figure 2 of the main text, including ethanol (top traces) and a series of odd-numbered carbon compounds (i.e., $\text{C}_9\text{H}_{18}\text{O}$, $\text{C}_{11}\text{H}_{22}\text{O}$, $\text{C}_{13}\text{H}_{26}\text{O}$ and $\text{C}_{15}\text{H}_{30}\text{O}$) characteristic of *zwf1* (heatmap).

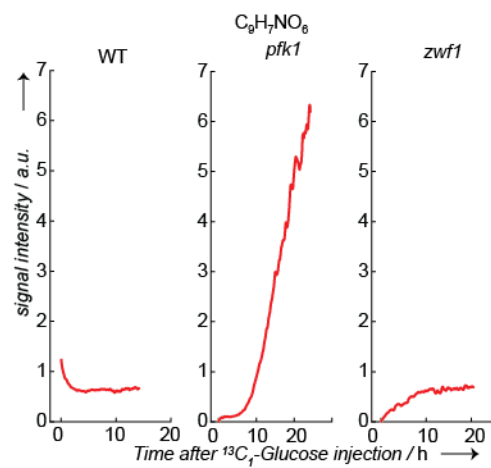


Figure S4. One selected compound detected in excess in mutant *pfk1*.

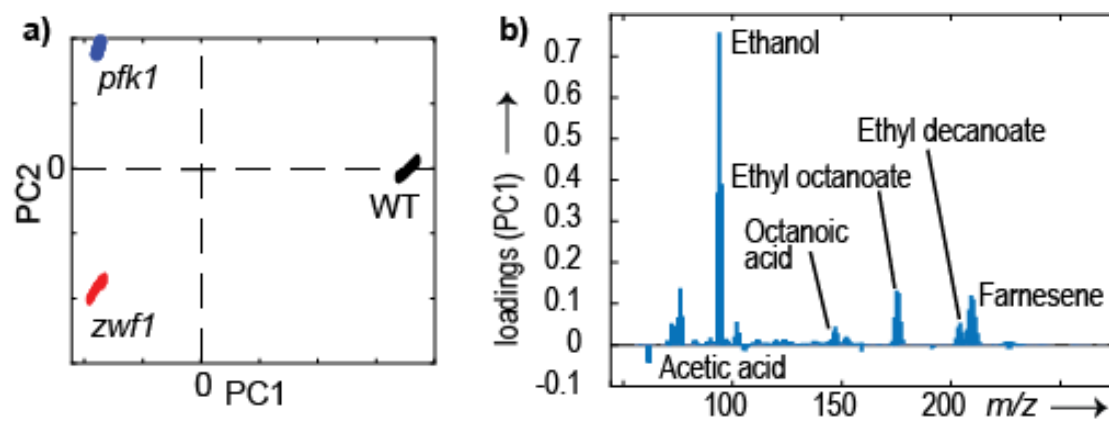


Figure S5. PCA including ethanol and acetic acid.

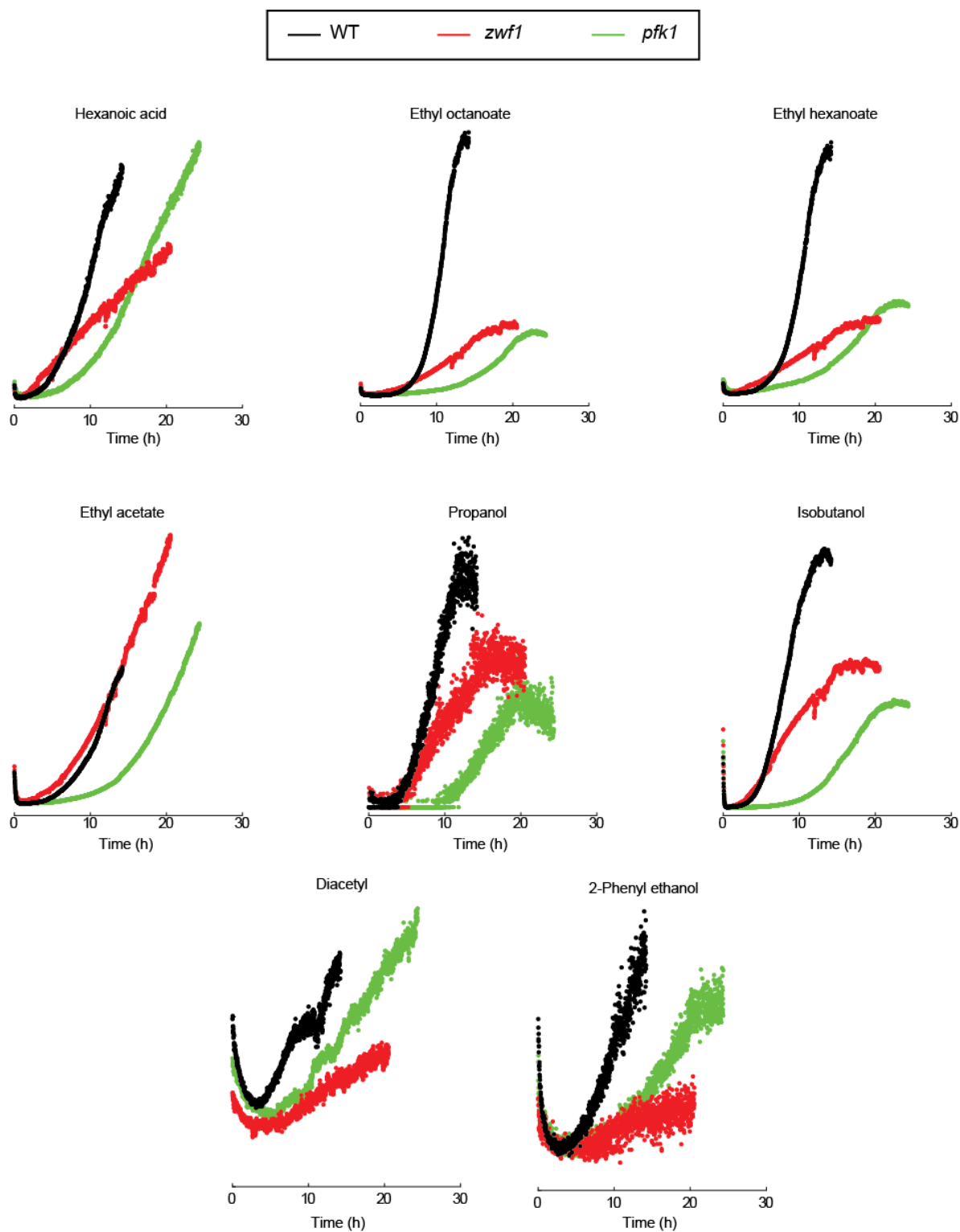


Figure S6. Aroma-relevant compounds were produced at different rates for the three strains investigated. Note that the bottom five compounds were not confirmed via MS/MS and thus assignment is only based on accurate mass and isotopic distribution.

Supporting Information

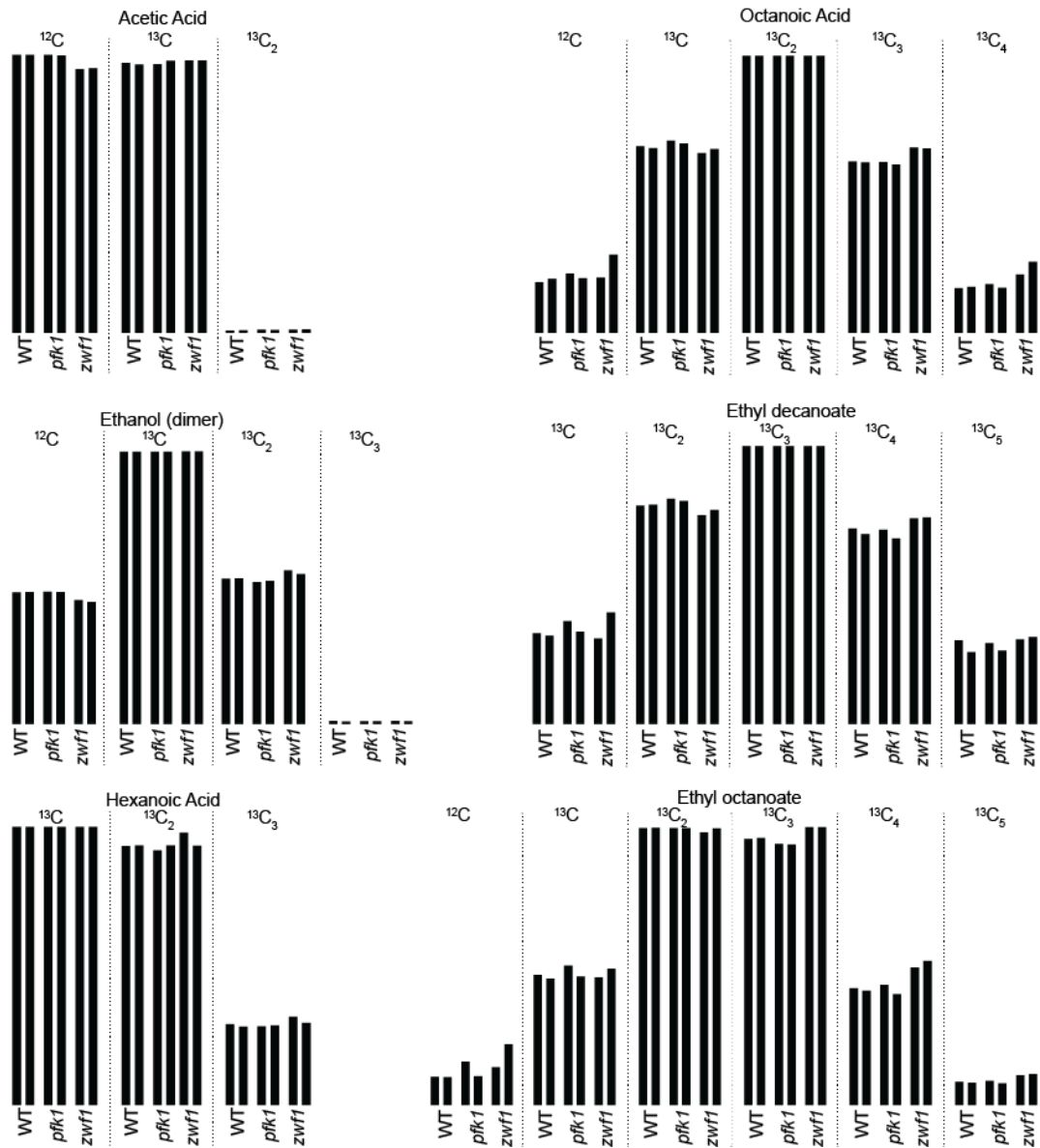


Figure S7. Replicate experiment confirmed enhanced incorporation of ^{13}C in metabolites of *zwf1* as compared to WT and *pfk1*.

Supporting Information

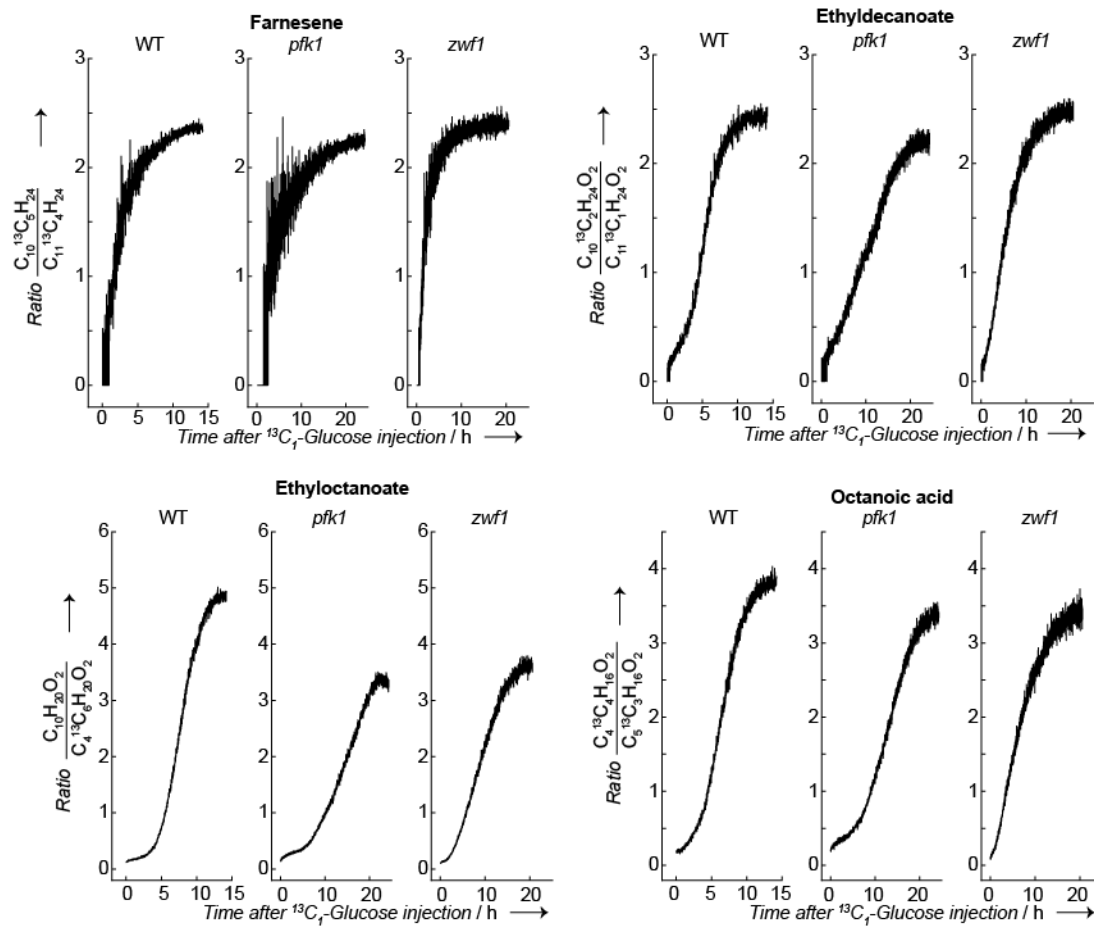


Figure S8. $^{13}\text{C}/^{12}\text{C}$ ratios for identified compounds show the kinetics of volatiles production upon $^{13}\text{C}_1$ -glucose injection.

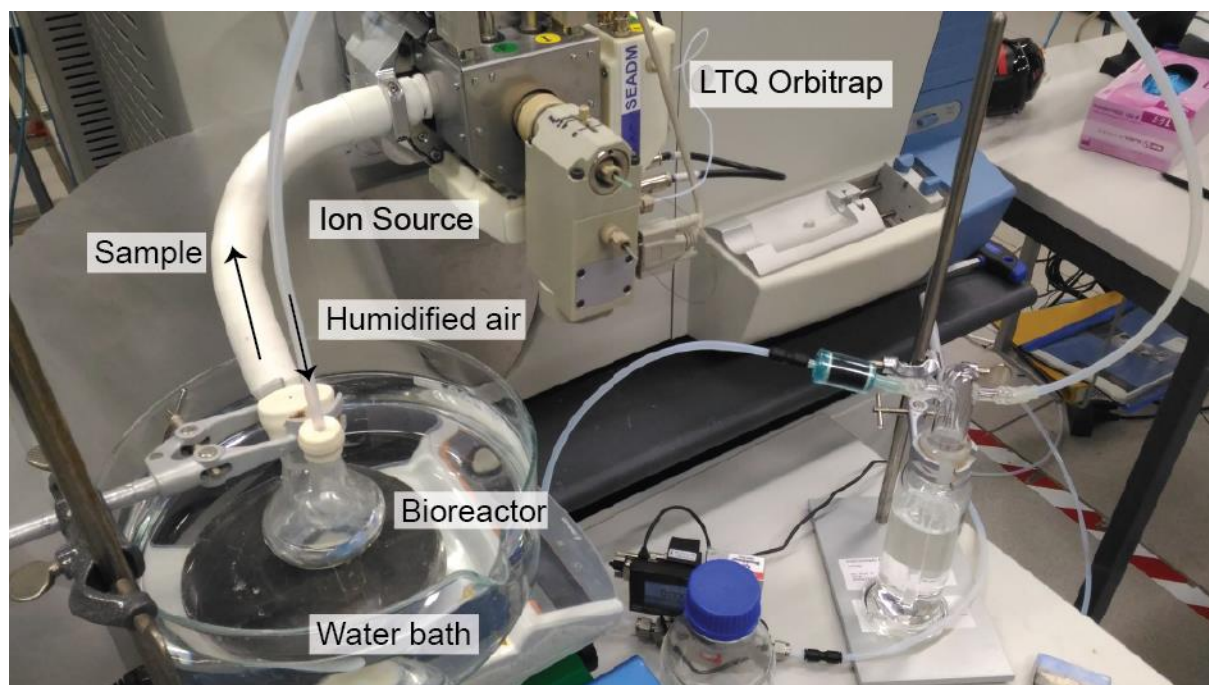


Figure S9. Experimental set-up used to monitor yeast volatiles during growth in glucose.

Supporting Information

Table S1 263 signals detected upon injecting $^{13}\text{C}_6$ -glucose and ^{12}C -glucose to WT. The order corresponds to the one shown in the heatmap from Figure 1b (top-to-bottom). Note how series of molecules with similar molecular formula tend to cluster together. The molecular *formulae* were generated assuming $[\text{M}+\text{H}]^+$ ion formation.

#	Molecular formula		Match with databases*	m/z measured with ¹² C-glucose	error (ppm)	m/z measured with ¹³ C ₆ -glucose	Mass error (ppm)	RDBE	S/N**
1	C2H6O2	YMDB01564	Ethylene glycol	63.0440	-0.2	65.0506	-1.8	0	4.0E+03
2	C10H10O2	YMDB01744	Methyl cinnamate	163.0754	0.1	173.1088	-0.4	6	5.1E+04
3	C8H6O	HMDB32929	Benzofuran	119.0486	-4.8	127.0754	-4.3	6	7.3E+02
4	C8H8N2	HMDB33171	1-Methylpyrrolo[1,2-a]pyrazine	133.0759	-0.8	141.1032	2.6	6	2.8E+02
5	C8H8O4	YMDB01802	Vanillic acid	169.0495	-0.4	177.0763	-0.3	5	6.1E+00
6	C11H10O3	HMDB40938	Coixinden A	191.0705	1.1	202.1074	1.5	7	3.4E+01
7	C8H3NO2	HMDB31004	Diatretin 2	146.0236	-0.5	154.0500	-3.2	8	2.2E+01
8	C11H9NO2	HMDB00734	Indoleacrylic acid	188.0707	0.3	199.1076	0.8	8	2.1E+01
9	C11H9NO			172.0757	0.1	183.1126	0.6	8	8.2E+00
10	C11H11NO	HMDB32887	4-Amino-2-methyl-1-naphthol	174.0908	-3.1	185.1286	2.5	7	5.0E+01
11	C12H9NO	JP007862	PHENYL 2-PYRIDYL KETONE	184.0754	-1.6	196.1163	2.1	9	4.0E+01
12	C11H5NO			168.0450	3.9	179.0820	4.2	10	2.6E+02
13	C8H8N2O2	HMDB42006	Ricinine	165.0658	-0.1	173.0922	-2.5	6	7.4E+01
14	C19H24			253.1951	0.3	272.2580	-2.6	8	6.7E+00
15	C8H8O3	YMDB01803	Vanillin	153.0545	-0.8	161.0809	-3.4	5	1.4E+02
16	C8H7NO5	HMDB62403	4-hydroxy-3-nitrophenylacetate	198.0396	-0.6	206.0655	-4.9	6	1.0E+02
17	C9H6O5			195.0286	-1.2	204.0585	-2.4	7	1.7E+03
18	C14H10O3	HMDB33925	Oroselone	227.0700	-1.2	241.1180	3.2	10	4.0E+01
19	C14H12O3	YMDB01780	Resveratrol	229.0860	0.4	243.1335	2.8	9	2.8E+00
20	C11H14	HMDB61808	(3-Methyl-2-butenyl)-benzene	147.1167	-0.8	158.1541	2.6	5	1.2E+04
21	C7H19N5O4			238.1517	3.2	245.1746	0.7	1	4.9E+01
22	C11H10O2	HMDB31845	3-Propylidene-1(3H)-isobenzofuranone	175.0755	0.9	186.1125	1.3	7	2.5E+01
23	C11H9NO3	YMDB00169	3-(indol-3-yl)pyruvic acid	204.0656	0.5	215.1026	0.9	8	2.4E+00
24	C11H8O5	HMDB30789	Dracunculin	221.0444	-0.3	232.0818	2.1	8	6.6E+00
25	C8H11NO4			186.0762	0.4	194.1021	-4.1	4	1.5E+00
26	C8H3NO			130.0282	-4.4	138.0550	-3.9	8	2.5E+01

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27	C7H14O	YMDB01337	2-Heptanone	115.1116	-1.7	122.1353	0.9	1	Inf
28	C6H12	HMDB29597	Cyclohexane	85.1013	2.0	91.1211	-1.6	1	1.3E+06
29	C19H28O2	HMDB36205	alpha-Amylcinnamyl isovalerate	289.2162	-0.1	308.2795	-1.2	6	2.1E+04
30	C10H16O3	HMDB36998	(S)-Oleuropeic acid	185.1174	1.2	195.1509	0.7	3	2.7E+02
31	C10H18O3	YMDB16206	3-Oxodecanoic acid	187.1330	0.7	197.1664	0.2	2	3.5E+04
32	C10H18O	YMDB01760	Nerol	155.1431	0.2	165.1765	-0.3	2	Inf
33	C5H8	C16521	Isoprene	69.0701	3.3	74.0868	2.5	2	9.0E+07
34	C7H6			91.0544	1.7	98.0777	0.0	5	1.0E+07
35	C9H3NO3			174.0187	0.7	183.0481	-3.2	9	7.7E+01
36	C9H10O3	YMDB01687	Ethyl vanillin	167.0702	-0.4	176.1001	-1.9	5	7.5E+01
37	C5H8O3	YMDB00365	Alpha-Ketoisovaleric acid	117.0545	-0.8	122.0712	-1.1	2	5.3E+02
38	C11H22O	YMDB01592	2-Undecanone	171.1743	-0.1	182.2113	0.4	1	5.8E+05
39	C16H32O2	YMDB00069	Palmitic acid	257.2478	1.0	273.3014	1.1	1	2.5E+04
40	C7H16O2	HMDB37636	xi-1-Butoxy-1-methoxyethane	133.1225	1.6	140.1458	0.4	0	5.0E+07
41	C4H10O	YMDB00573	isobutanol	75.0805	0.4	79.0941	3.4	0	3.3E+14
42	C4H12O2	YMDB00883	Ethanol (dimer)	93.0910	-0.2	97.1046	2.2	-1	4.2E+10
43	C3H8O	YMDB01718	Isopropanol	61.0648	-0.2	64.0749	0.8	0	6.2E+06
44	C5H14O2			107.1067	0.2	112.1234	-0.2	-1	3.5E+06
45	C12H24O2	YMDB01391	Ethyl decanoate	201.1854	2.6	213.2250	-0.5	1	6.3E+08
46	C9H24N4O			205.2027	1.8	214.2317	-3.7	0	3.5E+11
47	C5H10	JP005997	Cyclopentane	71.0857	1.8	76.1024	1.1	1	Inf
48	C7H18O2			135.1381	0.8	142.1614	-0.2	-1	2.3E+07
49	C14H28O2	YMDB01332	Ethyl dodecanoate	229.2164	0.7	243.2634	1.3	1	2.8E+07
50	C6H14O2	YMDB01709	Hexanediol	119.1068	1.4	125.1266	-1.2	0	Inf
51	C4H6N2O	HMDB60768	4-Hydroxymethylpyrazole	99.0557	3.8	103.0689	1.6	3	3.8E+04
52	C4H10N2O			103.0868	1.8	107.1004	3.9	1	Inf
53	C4H9N	HMDB31641	Pyrrolidine	72.0807	-1.6	76.0943	1.6	1	Inf
54	C17H30O	HMDB31336	(Z)-9-Cycloheptadecen-1-one	251.2374	1.8	268.2946	2.5	3	Inf
55	C18H28O2	HMDB06547	Stearidonic acid	277.2165	1.0	295.2767	0.7	5	Inf
56	C10H23NO2			190.1803	0.8	200.2137	0.3	0	3.8E+04
57	C11H22O2	YMDB01351	Isopentyl hexanoate	187.1693	0.2	198.2062	0.6	1	Inf

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58	C10H20O2	YMDB01389	Ethyl octanoate	173.1540	2.5	183.1875	1.9	1	Inf
59	C6H16O2	YMDB01718	Isopropanol (dimer)	121.1224	0.6	127.1426	1.6	-1	3.1E+03
60	C13H26O2	YMDB01364	Propyl decanoate	215.2007	0.6	228.2438	-1.5	1	9.5E+02
61	C12H27NO2			218.2117	1.1	230.2517	0.2	0	Inf
62	C18H31NO2			294.2427	-0.1	312.3021	-3.1	4	4.3E+01
63	C5H15N5O2			178.1304	3.3	183.1458	-4.4	1	9.0E+02
64	C20H38O4	JP001741	Octanedioic acid, dihexyl ester	343.2845	0.5	363.3522	2.5	2	Inf
65	C13H22N2O5			287.1612	3.7	300.2034	-1.0	4	1.1E+02
66	C18H34O4	HMDB00782	Octadecanedioic acid	315.2531	0.2	333.3138	1.4	2	1.1E+13
67	C12H20			165.1640	1.1	177.2040	-0.1	3	5.4E+04
68	C5H4			65.0385	-0.5	70.0553	-1.1	4	Inf
69	C8H16O2	YMDB00676	Octanoic acid	145.1222	-0.7	153.1490	-0.5	1	4.6E+09
70	C18H34O2	YMDB01368	Ethyl 9-hexadecenoate	283.2636	1.5	301.3238	1.3	2	Inf
71	C10H5NO5			220.0243	1.1	230.0568	-3.2	9	3.2E+04
72	C10H5NO2			172.0394	0.7	182.0719	-4.8	9	5.4E+02
73	C13H20	HMDB61825	1-Phenylheptane	177.1636	-0.7	190.2076	1.6	4	9.0E+05
74	C15H22	YMDB16091	alpha-Curcumene	203.1795	0.3	218.2296	-0.3	5	Inf
75	C15H24O	YMDB15971	Butylated hydroxytoluene	221.1900	0.0	236.2401	-0.5	4	Inf
76	C7H12			97.1010	-1.4	104.1248	1.6	2	Inf
77	C8H14O	YMDB01444	1-octen-3-one	127.1117	-0.4	135.1385	-0.2	2	Inf
78	C9H16	HMDB37777	2-Isopropyl-1,4-hexadiene	125.1324	-0.4	134.1628	1.1	2	Inf
79	C8H14	YMDB15921	1,3-Octadiene	111.1167	-0.9	119.1436	-0.6	2	Inf
80	C6H10	HMDB31544	3-Methylcyclopentene	83.0858	3.2	89.1056	-0.6	2	6.3E+08
81	C6H6	HMDB01505	Benzene	79.0542	0.1	85.0745	1.7	4	4.5E+05
82	C7H8	HMDB34168	Toluene	93.0699	0.6	100.0932	-0.9	4	2.1E+10
83	C12H18	HMDB13806	1,3-Diisopropylbenzene	163.1484	1.7	175.1884	0.5	4	7.9E+07
84	C15H29NO			240.2323	0.3	255.2828	1.5	2	Inf
85	C15H27N1			222.2222	2.5	237.2719	0.0	3	Inf
86	C7H10	HMDB31532	1-Methyl-1,3-cyclohexadiene	95.0855	-0.5	102.1092	2.6	3	6.4E+10
87	C8H12	HMDB61897	(Z)-1,3-Octadiene	109.1012	0.0	117.1280	0.2	3	Inf
88	C8H10	YMDB16013	Ethylbenzene	107.0856	0.9	115.1124	1.1	4	6.9E+04

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89	C15H24	YMDB16101	beta-Farnesene	205.1950	-0.2	220.2461	3.3	4	Inf
90	C11H16	HMDB61809	1-Methyl-4-(1-methylpropyl)-benzene	149.1327	1.5	160.1696	2.0	4	2.6E+09
91	C9H12	YMDB15979	Cumene	121.1013	1.2	130.1312	-0.9	4	3.7E+06
92	C15H26O	YMDB16053	Nerolidol	223.2060	1.6	238.2561	1.0	3	Inf
93	C9H14	HMDB38140	Santene	123.1169	0.4	132.1472	1.8	3	Inf
94	C10H14	YMDB16062	P-Cymene	135.1170	1.4	145.1504	0.7	4	Inf
95	C6H8			81.0698	-1.1	87.0900	0.5	3	Inf
96	C4H10O2	YMDB01407	2,3-butanediol	91.0754	0.8	95.0886	-1.4	0	7.2E+03
97	C2H5NO	YMDB01563	Acetamide	60.0447	4.9	62.0513	3.0	1	2.5E+08
98	C5H6	HMDB61878	Cyclopentadiene	67.0545	4.8	72.0713	3.9	3	1.7E+07
99	C10H5NO4			204.0289	-1.2	214.0623	-1.5	9	1.9E+05
100	C10H5NO3			188.0344	0.8	198.0669	-4.2	9	1.9E+07
101	C10H7NO2	HMDB00842	Quinaldic acid	174.0550	0.1	184.0879	-2.8	8	6.4E+03
102	C10H7NO	HMDB62189	1-nitrosonaphthalene	158.0600	-0.2	168.0939	2.0	8	5.9E+02
103	C10H16	YMDB01753	Myrcene	137.1326	0.7	147.1660	0.0	3	Inf
104	C11H10O4	HMDB29775	Vinyl caffeate	207.0654	1.2	218.1019	-0.5	7	2.5E+00
105	C9H10O	YMDB01619	4-Methylacetophenone	135.0803	-1.2	144.1102	-2.9	5	1.6E+02
106	C8H10O3	YMDB16081	Syringol	155.0701	-1.4	163.0964	-3.9	4	1.3E+00
107	C8H10O2	YMDB01798	Tyrosol	139.0751	-1.9	147.1015	-4.7	4	7.1E+01
108	C5H6O2	YMDB15931	2-Furanmethanol	99.0440	-0.4	104.0607	-0.8	3	2.7E+04
109	C5H8O4	YMDB00394	2-Acetolactate	133.0495	-0.3	138.0658	-3.9	2	5.3E+01
110	C4H10O3	HMDB61944	Trihydroxybutane	107.0704	1.1	111.0836	-0.8	0	9.8E+02
111	C7H15NO2	HMDB06831	3-Dehydroxycarnitine	146.1177	0.7	153.1405	-3.2	1	7.7E+04
112	C7H14	HMDB61895	2,4-Dimethyl-2-pentene	99.1166	-2.4	106.1403	0.6	1	Inf
113	C9H18O3	HMDB31513	(±)-3-Hydroxynonanoic acid	175.1329	-0.1	184.1632	1.0	1	4.3E+06
114	C13H22			179.1796	1.2	192.2227	-1.3	3	1.2E+04
115	C15H26O2	HMDB40281	Geranyl valerate	239.2005	-0.2	254.2506	-0.7	3	6.2E+04
116	C9H16O	YMDB01794	trans-2-Nonenal	141.1274	0.0	150.1573	-1.7	2	1.9E+07
117	C15H28O	HMDB32218	(+/-)-Dihydrofarnesol	225.2216	1.2	240.2712	-1.3	2	Inf
118	C10H18	HMDB61795	(S)-3,7-Dimethyl-1,6-octadiene	139.1481	0.0	149.1815	-0.6	2	Inf
119	C6H12O	YMDB01421	trans-3-hexen-1-ol	101.0959	-2.3	107.1161	-1.0	1	Inf

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120	C11H20O	YMDB01588	2-Methylisoborneol	169.1588	0.5	180.1957	1.0	2	Inf
121	C12H12	HMDB59764	2,6-Dimethyl-naphtalene	157.1008	-2.1	169.1413	-0.4	7	1.5E+02
122	C14H24	HMDB61832	1-Acetyl-2-methylcyclopentene	193.1953	1.4	207.2419	-0.1	3	Inf
123	C9H10	YMDB16095	alpha-Methylstyrene	119.0858	2.0	128.1152	-3.6	5	1.2E+04
124	C6H4	YMDB01430	2-methoxyphenol	77.0387	1.4	83.0589	2.9	5	2.6E+02
125	C15H26			207.2106	-0.7	222.2612	0.8	3	Inf
126	C15H30O2	YMDB16051	Methyl tetradecanoate	243.2321	0.9	258.2817	-1.4	1	9.1E+08
127	C11H18	HMDB61811	4-Methyl-2-methylene-1-(1-methylethylidene)-cyclohexane	151.1483	0.9	162.1848	-1.4	3	1.7E+08
128	C13H24	HMDB41081	(Z)-1,5-Tridecadiene	181.1952	0.7	194.2387	0.6	2	Inf
129	C9H18O2	YMDB01347	Propyl hexanoate	159.1379	-0.4	168.1678	-1.8	1	Inf
130	C10H16O	YMDB01455	trans,trans-2,4-decadienal	153.1275	0.9	163.1609	0.3	3	Inf
131	C9H16O2	YMDB01605	3-Methyl-4-octanolide	157.1223	0.3	166.1522	-1.3	2	1.8E+05
132	C15H20	HMDB59858	beta-Calacorene	201.1639	0.7	216.2145	2.2	6	Inf
133	C4H6	HMDB41792	1,3-Butadiene	55.0544	3.3	59.0676	-0.6	2	8.6E+06
134	C12H16	HMDB61814	1-(1-methylethenyl)-3-(1-methylethyl)-benzene	161.1324	-0.5	173.1729	1.1	5	1.1E+04
135	C20H34O	HMDB39827	Serratol	291.2685	0.8	311.3357	1.6	4	2.2E+04
136	C16H26	HMDB34498	(3E,7E)-4,8,12-Trimethyl-1,3,7,11-tridecatetraene	219.2107	0.0	235.2648	2.1	4	Inf
137	C20H32	HMDB36845	Cembrene	273.2580	1.0	293.3248	0.4	5	Inf
138	C10H16O2	HMDB36103	Geranic acid	169.1220	-1.6	179.1555	-2.0	3	Inf
139	C8H12O3	HMDB32232	2,5-Dimethyl-4-ethoxy-3(2H)-furanone	157.0861	0.9	165.1129	1.0	3	3.7E+06
140	C10H14O	YMDB01648	Carvone	151.1115	-1.4	161.1454	0.9	4	Inf
141	C7H14O2	YMDB01342	Ethyl pentanoate	131.1065	-1.1	138.1298	-2.1	1	1.6E+06
142	C6H8O3	YMDB01694	Furaneol	129.0547	0.4	135.0749	1.3	3	3.1E+04
143	C8H9NO3	HMDB01545	Pyridoxal	168.0657	0.8	176.0916	-4.2	5	8.6E+00
144	C8H11NO3	HMDB04817	5-Hydroxydopamine	170.0812	0.2	178.1076	-2.2	4	1.1E+01
145	C16H28O	HMDB36831	Ambronide	237.2217	1.7	253.2753	1.8	3	Inf
146	C16H30O2	YMDB00131	Oleic acid	255.2322	1.4	271.2859	1.5	2	Inf
147	C11H14O3	YMDB01809	Zingerone	195.1016	0.1	206.1385	0.5	5	3.1E+01
148	C7H10O2	YMDB16038	Lavander lactone	127.0754	0.4	134.0987	-0.7	3	3.6E+04
149	C11H12O3	HMDB35275	Isomyristicin	193.0860	0.6	204.1230	1.0	6	7.7E+00

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150	C3H8O3	YMDB00283	Glycerol	93.0547	0.8	96.0648	1.5	0	1.4E+03
151	C14H4N4O			245.0447	-4.6	259.0922	-2.0	15	1.6E+01
152	C18H36O2	YMDB01349	Ethyl hexadecanoate	285.2791	1.2	303.3394	0.9	1	Inf
153	C10H18O2	YMDB01611	3,7-Dimethyl-1,5-octadien-3,7-dio	171.1380	0.5	181.1715	0.0	2	8.3E+05
154	C7H12O2	YMDB01746	Methyl succinate	129.0910	-0.4	136.1138	-4.8	2	5.6E+03
155	C10H3NO4			202.0142	3.7	212.0463	-3.2	10	5.2E+05
156	C9H18O	YMDB01383	2-nonanone	143.1429	-0.7	152.1733	0.6	1	Inf
157	C7H12O	HMDB31540	4-Methylcyclohexanone	113.0960	-0.8	120.1193	-2.0	2	Inf
158	C10H12	YMDB15981	Dehydro-p-cymene	133.1010	-1.3	143.1344	-1.7	5	Inf
159	C9H14O	YMDB01795	trans-2,4-Nonaidenal / nona-2,6-dienal	139.1118	0.7	148.1417	-1.1	3	Inf
160	C6H8O	YMDB01437	2-ethylfuran	97.0648	-0.4	103.0850	0.9	3	1.5E+04
161	C12H22O2	YMDB01366	Ethyl 9-decenoate	199.1694	0.9	211.2090	-2.2	2	8.1E+05
162	C6H10O3	YMDB16200	3-Oxohexanoic acid	131.0702	-0.4	137.0905	0.6	2	1.6E+07
163	C6H8O2	YMDB01784	Sorbic acid	113.0597	0.0	119.0799	1.1	3	1.1E+05
164	C8H13NO	HMDB37868	2,4-Dimethyl-5-propyloxazole	140.1068	-1.1	148.1337	-0.9	3	2.2E+05
165	C14H24O	JP008396	Ethyl geranyl acetone	209.1903	1.5	223.2374	2.1	3	9.8E+05
166	C14H26O2	YMDB16214	trans-Tetra-dec-2-enoic acid	227.2008	1.1	241.2474	-0.1	2	2.0E+06
167	C5H13NO2			120.1018	-0.6	125.1185	-0.9	0	Inf
168	C10H12O2	YMDB01472	Phenylethyl acetate	165.0909	-0.5	175.1243	-0.9	5	Inf
169	C6H10O	YMDB01707	Hexa-2,4-dienol	99.0803	-1.4	105.1005	-0.1	2	Inf
170	C15H22O	HMDB36071	Dendrolasin	219.1744	0.5	234.2246	-0.1	5	3.3E+07
171	C15H20O	HMDB38147	Isogermafurene	217.1589	0.9	232.2090	0.3	6	2.7E+04
172	C11H16O	HMDB31866	2-Methyl-4-phenyl-2-butanol	165.1272	-1.1	176.1642	-0.5	4	4.4E+04
173	C13H18	HMDB61824	1-Methyl-4-(1-methyl-2-propenyl)-benzene	175.1481	-0.2	188.1916	-0.3	5	Inf
174	C11H12			145.1012	-0.2	156.1381	0.4	6	4.2E+03
175	C11H16O2	YMDB15988	Dihydroactinidiolide	181.1222	-0.7	192.1591	-0.2	4	2.1E+03
176	C10H14O2	YMDB15989	Dihydroeugenol	167.1065	-1.0	177.1399	-1.4	4	Inf
177	C9H14O3	HMDB30471	1,4-Ipomeadiol	171.1018	1.1	180.1316	-0.4	3	Inf
178	C16H24	HMDB36578	Cyperotundone	217.1952	0.4	233.2488	0.6	5	Inf
179	C6H15NO2			134.1175	-0.2	140.1378	0.7	0	Inf
180	C4H11NO2	YMDB01327	2-Amino-2-methyl-1,3-propanediol	106.0861	-1.1	110.0998	1.1	0	5.0E+05

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181	C5H12O2	YMDB01423	3-ethoxy-1-propanol	105.0911	1.2	110.1078	0.7	0	1.1E+07
182	C6H12O3	YMDB01419	Ethyl 4-hydroxybutanoate	133.0858	-1.1	139.1060	-0.1	1	1.1E+07
183	C5H13NO3			136.0968	-0.2	141.1135	-0.5	0	4.1E+04
184	C5H10O3	YMDB01429	Ethyl 2-hydroxy propanoate	119.0705	2.2	124.0868	-1.8	1	3.8E+06
185	C5H8O2	YMDB01434	2,3-pentanedione	101.0600	3.1	106.0767	2.6	2	2.7E+09
186	C4H8O2	YMDB00410	(R)-Acetoin	89.0599	2.0	93.0731	-0.4	1	2.2E+07
187	C5H6O3	HMDB31859	Norfuraneol	115.0390	0.0	120.0557	-0.3	3	5.2E+05
188	C3H8O2	YMDB01405	propylene glycol	77.0597	0.4	80.0699	1.2	0	Inf
189	C3H6O	YMDB00911	Propanal	59.0492	1.4	62.0593	2.4	1	2.7E+06
190	C2H5NO2	YMDB00016	Glycine	76.0396	4.5	78.0462	3.0	1	4.5E+03
191	C15H24O2	HMDB02352	Capsidiol	237.1850	0.2	252.2355	1.5	4	7.1E+13
192	C14H22	HMDB59739	1-Ethyl-3,5-diisopropyl-benzene	191.1793	-0.5	205.2259	-1.9	4	Inf
193	C10H10O	YMDB01440	2-phenylbut-2-enal	147.0804	-0.2	157.1138	-0.7	6	2.3E+03
194	C16H26O	HMDB40179	2,6-Di-tert-butyl-4-ethylphenol	235.2057	0.2	251.2598	2.2	4	Inf
195	C16H28O2	HMDB00477	7Z,10Z-Hexadecadienoic acid	253.2162	0.0	269.2699	0.2	3	Inf
196	C5H10O	YMDB00485	2-Methylbutanal	87.0806	2.0	92.0973	1.4	1	Inf
197	C6H6O	YMDB16074	Phenol	95.0492	0.6	101.0694	1.8	4	8.9E+03
198	C10H12O	YMDB01637	Anethole	149.0960	-0.8	159.1294	-1.3	5	3.7E+04
199	C7H10O	HMDB40278	2-Isopropylfuran	111.0804	0.0	118.1037	-1.2	3	Inf
200	C8H14O2	YMDB01365	Ethyl 2-hexenoate	143.1067	0.0	151.1335	0.1	2	3.2E+06
201	C8H14O3	YMDB16204	3-Oxo-octanoic acid	159.1016	0.3	167.1284	0.4	2	4.8E+05
202	C8H12O	YMDB15959	6-Methyl-3,5-heptadiene-2-one	125.0961	0.4	133.1230	0.5	3	1.2E+04
203	C7H8O	YMDB01730	m-Cresol	109.0649	0.9	116.0882	-0.4	4	Inf
204	C9H14O2	HMDB40285	Anapear	155.1068	0.9	164.1367	-0.7	3	2.4E+04
205	C11H14O	HMDB41493	4-Isopropylphenylacetaldehyde	163.1117	-0.5	174.1486	0.1	5	9.1E+02
206	C9H12O2	YMDB01615	4-Ethyl-2-methoxyphenol	153.0908	-1.4	162.1207	-2.9	4	7.4E+03
207	C12H14			159.1168	0.1	171.1569	-1.0	6	2.2E+04
208	C15H22O2	HMDB36427	Procurcumenol	235.1694	0.6	250.2195	0.1	5	1.2E+06
209	C9H12O	YMDB15966	Benzenepropanol	137.0958	-1.9	146.1262	-0.5	4	4.9E+03
210	C10H10			131.0855	-0.5	141.1193	2.1	6	Inf
211	C9H12O3	YMDB01712	Homovanillyl alcohol	169.0858	-1.0	178.1161	0.1	4	2.7E+03

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212	C15H20O2	HMDB36688	Costunolide	233.1538	1.0	248.2044	2.3	6	6.7E+03
213	C10H12O3	HMDB11751	3-Methoxybenzenepropanoic acid	181.0863	2.3	191.1193	-0.6	5	1.4E+01
214	C10H14O3	YMDB16019	Isoamyl 2-furoate	183.1014	-0.7	193.1349	-1.1	4	4.5E+01
215	C20H38O2	HMDB35159	Paullinic acid	311.2950	1.7	331.3618	1.1	2	Inf
216	C15H31NO			242.2483	1.7	257.2984	1.1	1	1.7E+08
217	C16H33NO2			272.2589	1.9	288.3126	1.9	1	Inf
218	C18H32O2	YMDB00884	Linoleic acid	281.2480	1.9	299.3069	-2.9	3	3.3E+06
219	C8H16O	YMDB01352	1-Octen-3-ol	129.1272	-1.1	137.1545	2.4	1	4.4E+03
220	C9H10O2	YMDB01624	4-Vinylguaiaicol	151.0752	-0.8	160.1051	-2.3	5	5.6E+01
221	C3H7NO2	YMDB00154	L-Alanine	90.0549	-0.8	93.0646	-4.9	1	1.6E+02
222	C4H4O3	HMDB32523	Succinic anhydride	101.0233	-0.4	105.0365	-2.4	3	3.9E+02
223	C10H20O3	YMDB16207	(R)-3-Hydroxydecanoic acid	189.1486	0.2	199.1820	-0.2	1	6.1E+01
224	C7H3NO3			150.0184	-1.1	157.0426	3.7	7	3.9E+02
225	C3H6N2O2	HMDB14405	Cycloserine	103.0505	2.7	106.0606	3.3	2	5.6E+03
226	C9H16O3	HMDB60287	4-Hydroperoxy-2-nonenal	173.1173	0.5	182.1472	-0.9	2	1.2E+07
227	C13H22O	YMDB01701	Geranyl acetone	195.1746	1.4	208.2177	-1.0	3	9.5E+04
228	C12H20O	HMDB31181	Homodihydrojasmane	181.1589	1.2	193.1985	-2.2	3	3.6E+05
229	C6H10O2	YMDB01685	Ethyl lactate	115.0753	-0.8	121.0955	0.3	2	3.3E+09
230	C5H10O2	YMDB01390	Propyl acetate	103.0756	2.1	108.0923	1.6	1	1.1E+07
231	C3H6O2	YMDB01684	Ethyl formate	75.0442	1.7	78.0543	2.5	1	2.7E+06
232	C5H8O	HMDB31407	Cyclopentanone	85.0651	3.2	90.0818	2.5	2	8.1E+05
233	C4H8O	YMDB01335	Ethoxy ethene	73.0649	1.8	77.0781	-1.1	1	Inf
234	C4H6O2	YMDB16203	But-2-enoic acid	87.0443	3.1	91.0575	0.6	2	3.9E+03
235	C11H14O2	HMDB31864	Methyleugenol	179.1066	-0.2	190.1436	0.3	5	2.0E+01
236	C15H24O3	HMDB35729	Dihydromyoporone	253.1804	2.1	268.2300	-0.1	4	2.7E+03
237	C11H18O2	HMDB35156	Neryl formate	183.1377	-1.2	194.1747	-0.7	3	Inf
238	C6H12O2	YMDB01424	Hexanoic acid	117.0913	2.2	123.1110	-0.5	1	4.3E+09
239	C2H4O2	YMDB00056	Acetic acid	61.0285	1.4	63.0351	-0.4	1	7.8E+10
240	C4H6O	HMDB61873	3-Buten-2-one	71.0494	3.2	75.0626	0.1	2	8.6E+05
241	C14H20			189.1638	0.0	203.2104	-1.4	5	Inf
242	C15H22O3	HMDB36563	Valerenolic acid	251.1648	2.5	266.2140	-1.4	5	1.0E+03

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243	C15H24O4	HMDB36150	4,11,13,15-Tetrahydroidentin B	269.1749	0.5	284.2246	-1.5	4	6.8E+02
244	C5H12N2			101.1071	-2.7	106.1242	1.3	1	1.4E+05
245	C18H32O	HMDB37543	(±)-(Z)-2-(5-Tetradecenyl)cyclobutanone	265.2526	0.1	283.3129	-0.1	3	Inf
246	C11H14O4	HMDB13070	Sinapyl alcohol	211.0965	0.3	222.1330	-1.4	5	7.3E+00
247	C8H9NO4	HMDB00017	4-Pyridoxic acid	184.0606	1.0	192.0865	-3.6	5	3.5E+00
248	C16H31NO2			270.2434	2.2	286.2966	0.7	2	Inf
249	C4H9NO	HMDB31581	Morpholine	88.0756	-0.8	92.0893	1.8	1	1.6E+04
250	C14H22O	YMDB01634	alpha-Isomethyl-ionone	207.1743	-0.2	221.2214	0.5	4	2.5E+03
251	C13H16	YMDB01576	1,1,6-Trimethyl-1,2-dihydronaphthalene	173.1325	0.4	186.1756	-2.2	6	Inf
252	C8H8	YMDB16080	Styrene	105.0701	1.9	113.0964	-2.1	5	3.7E+04
253	C11H16O3	HMDB37725	Hexyl 2-furoate	197.1171	-0.4	208.1541	0.0	4	Inf
254	C15H22O4	HMDB30104	Humulinic acid A	267.1593	0.9	282.2086	-2.8	5	4.8E+02
255	C14H18			187.1482	0.6	201.1948	-0.9	6	9.4E+03
256	C11H18O3			199.1331	1.4	210.1696	-0.4	3	Inf
257	C15H26O4	HMDB40459	Ethylene brassylate	271.1904	0.2	286.2410	1.3	3	3.7E+02
258	C15H29NO4	HMDB00791	L-Octanoylcarnitine	288.2158	-4.0	303.2673	0.2	2	7.0E+02
259	C13H24O	HMDB41490	Dihydrogeranylacetone	197.1897	-1.4	210.2332	-1.4	2	Inf
260	C11H18O	HMDB36190	2-Heptylfuran	167.1432	1.1	178.1797	-1.0	3	Inf
261	C11H20O2	YMDB16108	gamma-Undecalactone	185.1537	0.7	196.1907	1.1	2	Inf
262	C13H24O2	HMDB37226	Citronellyl propionate	213.1851	1.0	226.2278	-3.1	2	2.2E+03
263	C17H32O	HMDB41335	8-Heptadecenal	253.2529	1.4	270.3097	0.4	2	Inf

*Matching formula with at least one compound of the yeast or human metabolome databases.

**Signal-to-noise ratio computed as the ratio of the variances of the signals of the experiment with yeast and the negative control where we spiked glucose into sterile medium (see example in Figure S1).

Table S2 Mass spectral features detected upon injecting $^{13}\text{C}_1$ -glucose to WT, *zwf1* and *pfk1*. The order corresponds to the one shown in the heatmap from Figure 2d (top-to-bottom). The molecular formulae were generated assuming $[\text{M}+\text{H}]^+$ ion formation.

#	<i>m/z</i>	molecular formula (^{12}C & ^{13}C)	Unique molecular formula	Mass error (ppm)
1	269.0499	C11(13C)1H5N5O3	C12H5N5O3	0.04
2	270.0530	C10(13C)2H5N5O3	C12H5N5O3	-1.01
3	268.0464	C12H5N5O3	C12H5N5O3	-0.58
4	149.0870	C8(13C)2H10O	C10H10O	-0.95
5	138.1034	C3(13C)2H13NO3	C5H13NO3	-1.07
6	271.0457	C10(13C)3H5N3O4	C13H5N3O4	1.40
7	79.0663	C1(13C)2H8O2	C3H8O2	-1.07
8	148.0835	C9(13C)1H10O	C10H10O	-2.09
9	227.0386	C8(13C)1H7NO6	C9H7NO6	2.97
10	226.0356	C9H7NO6	C9H7NO6	4.24
11	228.0422	C7(13C)2H7NO6	C9H7NO6	3.69
12	228.0314	C5(13C)4H5NO6	C9H5NO6	-4.29
13	108.0197	-	-	-
14	209.0277	C8(13C)1H5NO5	C9H5NO5	1.32
15	77.0427	C1(13C)1H5NO2	C2H5NO2	0.71
16	215.1554	C10(13C)2H20O3	C12H20O3	0.92
17	192.0480	C8(13C)1H6N2O3	C9H6N2O3	-2.41
18	200.1640	C9(13C)3H20O2	C12H20O2	1.60
19	199.1605	C10(13C)2H20O2	C12H20O2	0.77
20	172.1326	C7(13C)3H16O2	C10H16O2	1.34
21	74.0317	C2(13C)1H4O2	C3H4O2	-0.79
22	176.0911	C5(13C)3H12O4	C8H12O4	1.33
23	170.0530	C7(13C)1H8O4	C8H8O4	0.55

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24	168.0733	C8(13C)1H10O3	C9H10O3	-2.13
25	202.1155	C9(13C)1H16O4	C10H16O4	-0.06
26	109.0559	C5(13C)2H6O	C7H6O	0.73
27	102.0268	C3(13C)1H4O3	C4H4O3	1.26
28	192.1676	C9(13C)1H22O3	C10H22O3	0.54
29	191.1641	C10H22O3	C10H22O3	-0.33
30	201.1120	C10H16O4	C10H16O4	-0.89
31	160.0684	C6(13C)1H10O4	C7H10O4	-0.90
32	236.1129	C7(13C)3H16O6	C10H16O6	3.66
33	159.0653	C7H10O4	C7H10O4	0.88
34	167.0612	C7(13C)2H8O3	C9H8O3	-0.57
35	186.0842	C8(13C)1H12O4	C9H12O4	0.22
36	105.0459	C2(13C)2H6O3	C4H6O3	1.90
37	133.0405	C3(13C)2H6O4	C5H6O4	-0.49
38	103.0299	C2(13C)2H4O3	C4H4O3	-1.51
39	190.1337	C5(13C)5H16O3	C10H16O3	-1.53
40	201.1030	C8(13C)2H14O4	C10H14O4	-0.99
41	183.0925	C8(13C)2H12O3	C10H12O3	-0.80
42	71.0404	C2(13C)2H4O	C4H4O	2.90
43	168.1015	C7(13C)3H12O2	C10H12O2	2.53
44	154.0858	C6(13C)3H10O2	C9H10O2	2.47
45	131.0886	C3(13C)4H10O2	C7H10O2	-1.41
46	143.0887	C4(13C)4H10O2	C8H10O2	-0.31
47	107.0525	(13C)4H6O3	C4H6O3	0.77
48	126.0629	C6(13C)1H8O2	C7H8O2	-1.10
49	91.0391	C3H6O3	C3H6O3	1.93
50	148.0597	C3(13C)3H8O4	C6H8O4	0.99
51	113.0508	C4(13C)2H6O2	C6H6O2	-0.14
52	100.0475	C4(13C)1H6O2	C5H6O2	1.27
53	172.1048	C8(13C)1H14O3	C9H14O3	-0.59
54	138.0631	C7(13C)1H8O2	C8H8O2	0.02

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55	104.0424	C3(13C)1H6O3	C4H6O3	0.31
56	154.0580	C7(13C)1H8O3	C8H8O3	0.31
57	76.0392	C2H5NO2	C2H5NO2	-1.49
58	171.0475	C4(13C)4H6O4	C8H6O4	1.41
59	163.0870	C9H10N2O	C9H10N2O	2.68
60	161.0710	C9H8N2O	C9H8N2O	0.52
61	70.0651	C4H7N	C4H7N	-0.27
62	188.1276	C7(13C)3H16O3	C10H16O3	1.47
63	187.1240	C8(13C)2H16O3	C10H16O3	0.59
64	186.1205	C9(13C)1H16O3	C10H16O3	-0.31
65	173.1083	C7(13C)2H14O3	C9H14O3	0.38
66	169.1135	C8(13C)2H14O2	C10H14O2	0.95
67	144.0734	C6(13C)1H10O3	C7H10O3	-1.32
68	131.0613	C4(13C)2H8O3	C6H8O3	-0.51
69	114.0632	C5(13C)1H8O2	C6H8O2	1.50
70	145.0770	C5(13C)2H10O3	C7H10O3	-0.16
71	115.0663	C4(13C)2H8O2	C6H8O2	-0.98
72	101.0506	C3(13C)2H6O2	C5H6O2	-1.56
73	89.0509	C2(13C)2H6O2	C4H6O2	1.73
74	219.0477	C8(13C)4H6O4	C12H6O4	1.61
75	133.0768	C4(13C)2H10O3	C6H10O3	-1.23
76	132.0737	C5(13C)1H10O3	C6H10O3	0.91
77	141.1184	C7(13C)2H14O	C9H14O	-0.18
78	129.0820	C5(13C)2H10O2	C7H10O2	-0.53
79	115.1026	C5(13C)2H12O	C7H12O	-1.83
80	147.0925	C5(13C)2H12O3	C7H12O3	-0.81
81	146.0894	C6(13C)1H12O3	C7H12O3	1.13
82	101.0873	C4(13C)2H10O	C6H10O	1.95
83	157.1134	C7(13C)2H14O2	C9H14O2	0.13
84	155.0978	C7(13C)2H12O2	C9H12O2	0.75
85	113.0870	C5(13C)2H10O	C7H10O	-1.01

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86	99.0713	C4(13C)2H8O	C6H8O	-1.60
87	97.0558	C4(13C)2H6O	C6H6O	-0.64
88	156.0736	C7(13C)1H10O3	C8H10O3	-0.31
89	160.0962	C5(13C)3H12O3	C8H12O3	1.18
90	159.0927	C6(13C)2H12O3	C8H12O3	0.14
91	158.0891	C7(13C)1H12O3	C8H12O3	-0.92
92	146.0805	C4(13C)3H10O3	C7H10O3	0.99
93	142.0942	C7(13C)1H12O2	C8H12O2	-1.35
94	145.1043	C4(13C)4H12O2	C8H12O2	-0.97
95	144.1012	C5(13C)3H12O2	C8H12O2	0.99
96	147.1198	C4(13C)4H14O2	C8H14O2	-1.62
97	129.1093	C4(13C)4H12O	C8H12O	-1.45
98	162.1117	C5(13C)3H14O3	C8H14O3	0.57
99	161.1082	C6(13C)2H14O3	C8H14O3	-0.47
100	160.1051	C7(13C)1H14O3	C8H14O3	1.30
101	144.1102	C7(13C)1H14O2	C8H14O2	1.13
102	146.1168	C5(13C)3H14O2	C8H14O2	0.32
103	145.1132	C6(13C)2H14O2	C8H14O2	-0.83
104	127.1027	C6(13C)2H12O	C8H12O	-0.55
105	127.0664	C5(13C)2H8O2	C7H8O2	0.22
106	157.0771	C6(13C)2H10O3	C8H10O3	0.75
107	143.0977	C6(13C)2H12O2	C8H12O2	-0.17
108	141.0821	C6(13C)2H10O2	C8H10O2	0.51
109	125.0872	C6(13C)2H10O	C8H10O	0.22
110	85.0557	C3(13C)2H6O	C5H6O	-2.39
111	186.1120	C7(13C)3H14O3	C10H14O3	2.01
112	174.1119	C6(13C)3H14O3	C9H14O3	1.34
113	172.0963	C6(13C)3H12O3	C9H12O3	1.91
114	175.1235	C7(13C)2H16O3	C9H16O3	-2.75
115	167.0980	C8(13C)2H12O2	C10H12O2	1.54
116	151.1030	C8(13C)2H12O	C10H12O	1.40

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117	187.0878	C7(13C)2H12O4	C9H12O4	1.11
118	185.1085	C8(13C)2H14O3	C10H14O3	1.12
119	148.0687	C5(13C)1H10O4	C6H10O4	1.12
120	162.0840	C6(13C)1H12O4	C7H12O4	-1.49
121	169.0772	C7(13C)2H10O3	C9H10O3	1.53
122	171.0928	C7(13C)2H12O3	C9H12O3	0.95
123	143.0614	C5(13C)2H8O3	C7H8O3	0.52
124	173.0721	C6(13C)2H10O4	C8H10O4	0.95
125	139.0666	C6(13C)2H8O2	C8H8O2	1.22
126	174.0756	C5(13C)3H10O4	C8H10O4	1.90
127	159.0564	C5(13C)2H8O4	C7H8O4	0.75
128	155.0611	C6(13C)2H8O3	C8H8O3	-1.52
129	141.0454	C5(13C)2H6O3	C7H6O3	-1.99
130	125.0509	C5(13C)2H6O2	C7H6O2	1.00
131	158.0528	C6(13C)1H8O4	C7H8O4	-0.30
132	142.0579	C6(13C)1H8O3	C7H8O3	-0.66
133	172.0685	C7(13C)1H10O4	C8H10O4	-0.02
134	130.0577	C5(13C)1H8O3	C6H8O3	-1.80
135	106.0579	C3(13C)1H8O3	C4H8O3	-0.61
136	120.0373	C3(13C)1H6O4	C4H6O4	0.65
137	88.0474	C3(13C)1H6O2	C4H6O2	-0.16
138	87.0349	C2(13C)2H4O2	C4H4O2	-2.32
139	134.0803	C3(13C)3H10O3	C6H10O3	0.03
140	118.0854	C3(13C)3H10O2	C6H10O2	-0.36
141	117.1096	C3(13C)4H12O	C7H12O	1.06
142	158.0811	C5(13C)3H10O3	C8H10O3	4.66
143	142.1219	C6(13C)3H14O	C9H14O	1.00
144	116.0425	C4(13C)1H6O3	C5H6O3	1.49
145	98.0683	C5(13C)1H8O	C6H8O	1.29
146	96.0527	C5(13C)1H6O	C6H6O	2.32
147	175.0876	C6(13C)2H12O4	C8H12O4	0.38

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148	132.0648	C3(13C)3H8O3	C6H8O3	0.76
149	128.1058	C5(13C)3H12O	C8H12O	-2.76
150	140.0786	C7(13C)1H10O2	C8H10O2	-0.68
151	124.0837	C7(13C)1H10O	C8H10O	-1.13
152	84.0526	C4(13C)1H6O	C5H6O	0.97
153	125.0540	C4(13C)1H5N3O	C5H5N3O	1.07
154	135.0561	C3(13C)2H8O4	C5H8O4	-1.20
155	124.0505	C5H5N3O	C5H5N3O	-0.27
156	123.0474	(13C)4H6O4	C4H6O4	1.04
157	109.0595	C4(13C)1H5N3	C5H5N3	4.96
158	141.0490	C4(13C)1H5N3O2	C5H5N3O2	1.27
159	123.0385	C4(13C)1H3N3O	C5H3N3O	1.88
160	140.0455	C5H5N3O2	C5H5N3O2	0.09
161	122.0350	C5H3N3O	C5H3N3O	0.52
162	121.0319	(13C)4H4O4	C4H4O4	1.86
163	92.0422	C2(13C)1H6O3	C3H6O3	-1.19
164	108.0560	C5H5N3	C5H5N3	3.45
165	89.0420	(13C)4H4O2	C4H4O2	1.50
166	64.0476	C1(13C)1H6O2	C2H6O2	2.45
167	178.1703	C5(13C)5H20O2	C10H20O2	-0.44
168	177.1668	C6(13C)4H20O2	C10H20O2	-1.39
169	176.1637	C7(13C)3H20O2	C10H20O2	0.22
170	175.1606	C8(13C)2H20O2	C10H20O2	1.84
171	174.1571	C9(13C)1H20O2	C10H20O2	0.89
172	214.2254	C6(13C)9H24	C15H24	0.50
173	213.2219	C7(13C)8H24	C15H24	-0.28
174	155.1525	C5(13C)6H16	C11H16	-0.77
175	225.1947	C9(13C)6H22O	C15H22O	0.89
176	224.1916	C10(13C)5H22O	C15H22O	2.15
177	223.1881	C11(13C)4H22O	C15H22O	1.42
178	222.1846	C12(13C)3H22O	C15H22O	0.67

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179	230.2293	C8(13C)7H26O	C15H26O	0.75
180	229.2262	C9(13C)6H26O	C15H26O	1.99
181	228.2227	C10(13C)5H26O	C15H26O	1.27
182	168.1647	C7(13C)5H18	C12H18	-1.44
183	227.2102	C9(13C)6H24O	C15H24O	0.45
184	226.2067	C10(13C)5H24O	C15H24O	-0.28
185	209.2002	C9(13C)6H22	C15H22	2.89
186	225.2036	C11(13C)4H24O	C15H24O	0.97
187	208.1966	C10(13C)5H22	C15H22	2.10
188	227.2192	C11(13C)4H26O	C15H26O	0.54
189	140.1337	C5(13C)5H14	C10H14	0.86
190	127.1301	C5(13C)4H14	C9H14	-1.48
191	126.1270	C6(13C)3H14	C9H14	0.76
192	113.1144	C4(13C)4H12	C8H12	-2.06
193	225.2121	C13(13C)2H26O	C15H26O	-0.94
194	125.1235	C7(13C)2H14	C9H14	-0.57
195	112.1113	C5(13C)3H12	C8H12	0.46
196	111.1078	C6(13C)2H12	C8H12	-1.04
197	212.2188	C8(13C)7H24	C15H24	1.06
198	154.1494	C6(13C)5H16	C11H16	1.07
199	211.2153	C9(13C)6H24	C15H24	0.27
200	153.1459	C7(13C)4H16	C11H16	-0.02
201	126.1180	C4(13C)5H12	C9H12	0.60
202	210.2122	C10(13C)5H24	C15H24	1.62
203	125.1145	C5(13C)4H12	C9H12	-0.73
204	124.1114	C6(13C)3H12	C9H12	1.55
205	111.0988	C4(13C)4H10	C8H10	-1.22
206	128.1336	C4(13C)5H14	C9H14	-0.16
207	210.2041	C10(13C)4H23N	C14H23N	1.82
208	228.2137	C8(13C)7H24O	C15H24O	1.18
209	114.1179	C3(13C)5H12	C8H12	-0.57

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210	85.0834	C2(13C)4H8	C6H8	1.54
211	151.1303	C7(13C)4H14	C11H14	0.62
212	149.1237	C9(13C)2H14	C11H14	1.41
213	121.0924	C7(13C)2H10	C9H10	1.01
214	150.1358	C10(13C)1H16	C11H16	-0.35
215	122.1044	C8(13C)1H12	C9H12	-1.16
216	97.0831	C3(13C)4H8	C7H8	-1.86
217	110.0957	C5(13C)3H10	C8H10	1.35
218	96.0800	C4(13C)3H8	C7H8	1.09
219	208.2051	C12(13C)3H24	C15H24	0.03
220	207.2016	C13(13C)2H24	C15H24	-0.77
221	152.1424	C8(13C)3H16	C11H16	-1.12
222	151.1393	C9(13C)2H16	C11H16	0.75
223	209.2087	C11(13C)4H24	C15H24	0.83
224	123.1079	C7(13C)2H12	C9H12	0.21
225	223.1970	C13(13C)2H24O	C15H24O	1.50
226	206.1896	C12(13C)3H22	C15H22	0.50
227	205.1865	C13(13C)2H22	C15H22	1.89
228	224.2001	C12(13C)3H24O	C15H24O	0.23
229	207.1927	C11(13C)4H22	C15H22	-0.87
230	109.0922	C6(13C)2H10	C8H10	-0.17
231	95.0765	C5(13C)2H8	C7H8	-0.67
232	124.1204	C8(13C)1H14	C9H14	1.72
233	110.1047	C7(13C)1H12	C8H12	1.53
234	136.1201	C9(13C)1H14	C10H14	-0.72
235	96.0890	C6(13C)1H10	C7H10	1.30
236	82.0733	C5(13C)1H8	C6H8	0.98
237	138.1477	C4(13C)3H18O2	C7H18O2	-2.09
238	137.1447	C5(13C)2H18O2	C7H18O2	-0.03
239	136.1416	C6(13C)1H18O2	C7H18O2	2.06
240	93.0610	C5(13C)2H6	C7H6	0.36

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241	134.0530	C4(13C)1H8O4	C5H8O4	0.91
242	119.0531	C3(13C)1H7NO3	C4H7NO3	-1.39
243	74.0958	C2(13C)3H10	C5H10	2.40
244	73.0922	C3(13C)2H10	C5H10	0.13
245	72.0887	C4(13C)1H10	C5H10	-2.20
246	218.1745	C9(13C)3H22O3	C12H22O3	1.23
247	217.1710	C10(13C)2H22O3	C12H22O3	0.47
248	167.1616	C8(13C)4H18	C12H18	0.25
249	166.1581	C9(13C)3H18	C12H18	-0.76
250	165.1550	C10(13C)2H18	C12H18	0.96
251	149.1354	C4(13C)4H16O2	C8H16O2	-2.24
252	148.1323	C5(13C)3H16O2	C8H16O2	-0.34
253	147.1288	C6(13C)2H16O2	C8H16O2	-1.48
254	146.1257	C7(13C)1H16O2	C8H16O2	0.45
255	139.1302	C6(13C)4H14	C10H14	-0.34
256	99.0991	C3(13C)4H10	C7H10	1.77
257	138.1267	C7(13C)3H14	C10H14	-1.55
258	98.0956	C4(13C)3H10	C7H10	0.08
259	97.0921	C5(13C)2H10	C7H10	-1.65
260	84.0799	C3(13C)3H8	C6H8	-0.44
261	137.1236	C8(13C)2H14	C10H14	0.51
262	83.0768	C4(13C)2H8	C6H8	2.99
263	129.1183	C6(13C)2H14O	C8H14O	-1.29
264	81.0608	C4(13C)2H6	C6H6	-1.33
265	142.1493	C5(13C)5H16	C10H16	0.16
266	141.1458	C6(13C)4H16	C10H16	-1.02
267	140.1427	C7(13C)3H16	C10H16	1.00
268	139.1392	C8(13C)2H16	C10H16	-0.19
269	135.1081	C8(13C)2H12	C10H12	1.23
270	69.0611	C3(13C)2H6	C5H6	2.96
271	68.0576	C4(13C)1H6	C5H6	0.53

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272	130.1223	C5(13C)3H14O	C8H14O	3.47
273	108.0887	C7(13C)1H10	C8H10	-1.72
274	226.2161	C12(13C)3H26O	C15H26O	1.80
275	173.1536	C10H20O2	C10H20O2	-0.07
276	94.0735	C6(13C)1H8	C7H8	2.36
277	158.1169	C6(13C)3H14O2	C9H14O2	1.18
278	164.1515	C11(13C)1H18	C12H18	-0.05
279	120.0888	C8(13C)1H10	C9H10	-0.37
280	224.2091	C14(13C)1H26O	C15H26O	0.32
281	80.0578	C5(13C)1H6	C6H6	2.22
282	256.1900	C12(13C)3H24O3	C15H24O3	0.56
283	78.0418	C5(13C)1H4	C6H4	-2.29
284	145.1222	C8H16O2	C8H16O2	-0.69
285	221.1810	C13(13C)2H22O	C15H22O	-0.08
286	137.1146	C6(13C)4H12	C10H12	0.36
287	135.1381	C7H18O2	C7H18O2	0.83
288	206.1806	C10(13C)5H20	C15H20	0.41
289	205.1771	C11(13C)4H20	C15H20	-0.41
290	220.1686	C12(13C)3H20O	C15H20O	-0.93
291	222.1756	C10(13C)5H20O	C15H20O	0.58
292	221.1725	C11(13C)4H20O	C15H20O	1.86
293	204.1740	C12(13C)3H20	C15H20	0.98
294	131.1253	C4(13C)4H14O	C8H14O	1.28
295	123.0990	C5(13C)4H10	C9H10	0.04
296	156.0933	C6(13C)2H11NO2	C8H11NO2	2.09
297	155.0898	C7(13C)1H11NO2	C8H11NO2	1.03
298	153.0823	C7(13C)2H10O2	C9H10O2	1.39
299	137.0873	C7(13C)2H10O	C9H10O	1.23
300	139.1029	C7(13C)2H12O	C9H12O	0.51
301	111.0715	C5(13C)2H8O	C7H8O	-0.16
302	150.1183	C6(13C)5H12	C11H12	2.38

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303	221.1631	C9(13C)6H18O	C15H18O	-0.26
304	180.1652	C8(13C)5H18	C13H18	1.94
305	236.1635	C12(13C)3H20O2	C15H20O2	-0.67
306	218.1530	C12(13C)3H18O	C15H18O	-0.49
307	169.1409	C7(13C)4H16O	C11H16O	0.25
308	219.1655	C13(13C)2H20O	C15H20O	0.36
309	161.1234	C10(13C)2H14	C12H14	-0.62
310	160.1114	C9(13C)3H12	C12H12	1.03
311	129.1371	C3(13C)6H14	C9H14	1.13
312	167.1343	C9(13C)2H16O	C11H16O	0.95
313	179.1613	C9(13C)4H18	C13H18	-1.50
314	225.2319	C10(13C)6H26	C16H26	4.45
315	178.1587	C10(13C)3H18	C13H18	2.61
316	219.1565	C11(13C)4H18O	C15H18O	0.27
317	152.1339	C6(13C)5H14	C11H14	1.72
318	220.1600	C10(13C)5H18O	C15H18O	1.02
319	205.1682	C9(13C)6H18	C15H18	-0.50
320	141.1368	C4(13C)6H14	C10H14	-1.16
321	127.1215	C3(13C)6H12	C9H12	1.91
322	166.1491	C7(13C)5H16	C12H16	-0.88
323	112.1023	C3(13C)5H10	C8H10	0.28
324	203.1620	C11(13C)4H18	C15H18	2.28
325	198.1484	C9(13C)3H18O2	C12O18O2	2.10
326	138.0908	C6(13C)3H10O	C9H10O	2.43
327	136.1120	C9H13N	C9H13N	-0.41
328	150.1273	C8(13C)3H14	C11H14	2.52
329	122.0959	C6(13C)3H10	C9H10	2.37
330	238.1795	C12(13C)3H22O2	C15H22O2	0.82
331	183.1565	C8(13C)4H18O	C12H18O	0.48
332	181.1500	C10(13C)2H18O	C12H18O	1.12
333	226.2349	C9(13C)7H26	C16H26	3.17

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334	163.1390	C10(13C)2H16	C12H16	-1.20
335	207.1842	C9(13C)6H20	C15H20	1.21
336	204.1651	C10(13C)5H18	C15H18	0.88
337	148.1113	C8(13C)3H12	C11H12	0.16
338	223.1791	C9(13C)6H20O	C15H20O	1.33
339	147.1077	C9(13C)2H12	C11H12	-0.98
340	203.1705	C13(13C)2H20	C15H20	0.16
341	202.1585	C12(13C)3H18	C15H18	1.47
342	139.0939	C5(13C)4H10O	C9H10O	0.37
343	211.1884	C3(13C)12H18	C152H18	-0.01
344	143.1528	C4(13C)6H16	C10H16	1.33
345	181.1773	C9(13C)4H20	C13H20	0.47
346	180.1742	C10(13C)3H20	C13H20	2.05
347	226.1977	C8(13C)7H22O	C15H22O	-0.37
348	179.1738	C4(13C)6H20O2	C10H20O2	0.49
349	169.1682	C6(13C)6H18	C12H18	-0.44
350	100.1022	C2(13C)5H10	C7H10	-1.10
351	214.1434	C2(13C)11H14O2	C131H14O2	-0.78
352	182.1808	C8(13C)5H20	C13H20	1.39
353	183.1292	C9(13C)2H16O2	C11H16O2	1.12
354	224.1826	C1(13C)15H16	C16H16	-0.74
355	184.1601	C7(13C)5H18O	C12H18O	1.38
356	181.1410	C8(13C)4H16O	C12H16O	1.01
357	197.1449	C10(13C)2H18O2	C12H18O2	1.26
358	138.1182	C5(13C)5H12	C10H12	1.57
359	124.1325	C3(13C)3H16O2	C6H16O2	0.96
360	121.1224	C6H16O2	C6H16O2	0.57
361	127.0938	C4(13C)4H10O	C8H10O	-0.71
362	108.1008	C2(13C)3H12O2	C5H12O2	-2.60
363	123.1290	C4(13C)2H16O2	C6H16O2	-0.39
364	122.1259	C5(13C)1H16O2	C6H16O2	1.93

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365	59.0766	C2(13C)2H8	C4H8	-0.60
366	58.0735	C3(13C)1H8	C4H8	4.34
367	155.1614	C7(13C)4H18	C11H18	-0.64
368	212.2273	C10(13C)5H26	C15H26	-0.97
369	154.1579	C8(13C)3H18	C11H18	-1.73
370	232.2453	C8(13C)7H28O	C15H28O	2.27
371	211.2229	C3(13C)6H24N4O	C9H24N4O	2.20
372	130.1491	C4(13C)5H16	C9H16	-0.90
373	229.2347	C11(13C)4H28O	C15H28O	0.12
374	231.2413	C9(13C)6H28O	C15H28O	-0.39
375	230.2378	C10(13C)5H28O	C15H28O	-1.12
376	115.1304	C4(13C)4H14	C8H14	1.06
377	242.2106	C12(13C)3H26O2	C15H26O2	0.01
378	227.2281	C13(13C)2H28O	C15H28O	0.63
379	129.1461	C5(13C)4H16	C9H16	1.29
380	128.1425	C6(13C)3H16	C9H16	-0.01
381	114.1268	C5(13C)3H14	C8H14	-0.40
382	113.1233	C6(13C)2H14	C8H14	-1.88
383	76.0750	C1(13C)3H8O	C4H8O	2.35
384	73.0833	C1(13C)4H8	C5H8	-0.15
385	210.0397	C9H7NO5	C9H7NO5	0.06
386	195.0483	C8(13C)1H7NO4	C9H7NO4	0.69
387	244.2100	C10(13C)4H25NO2	C14H25NO2	3.39
388	196.1960	C9(13C)5H22	C14H22	-0.78
389	195.1930	C10(13C)4H22	C14H22	0.66
390	194.1895	C11(13C)3H22	C14H22	-0.19
391	87.0990	C2(13C)4H10	C6H10	0.39
392	242.2017	C10(13C)5H24O2	C15H24O2	-0.08
393	240.1951	C12(13C)3H24O2	C15H24O2	0.41
394	239.1915	C13(13C)2H24O2	C15H24O2	-0.29
395	127.1390	C7(13C)2H16	C9H16	-1.32

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396	86.0955	C3(13C)3H10	C6H10	-1.56
397	100.1112	C4(13C)3H12	C7H12	-0.89
398	99.1081	C5(13C)2H12	C7H12	1.97
399	101.1147	C3(13C)4H12	C7H12	0.77
400	85.0924	C4(13C)2H10	C6H10	1.78
401	61.0558	C1(13C)2H6O	C3H6O	-0.55
402	212.0557	C9H9NO5	C9H9NO5	1.73
403	205.1977	C8(13C)4H24O2	C12H24O2	-2.96
404	238.0429	C10(13C)1H8O6	C11H8O6	0.66
405	213.0588	C8(13C)1H9NO5	C9H9NO5	0.39
406	197.0638	C8(13C)1H9NO4	C9H9NO4	0.19
407	169.0687	C7(13C)1H9NO3	C8H9NO3	-0.88
408	196.0603	C9H9NO4	C9H9NO4	-0.66
409	168.0657	C8H9NO3	C8H9NO3	0.80
410	234.2331	C9(13C)5H28O2	C14H28O2	0.42
411	233.2296	C10(13C)4H28O2	C14H28O2	-0.29
412	232.2265	C11(13C)3H28O2	C14H28O2	0.92
413	231.2230	C12(13C)2H28O2	C14H28O2	0.21
414	206.2012	C7(13C)5H24O2	C12H24O2	-2.14
415	204.1951	C9(13C)3H24O2	C12H24O2	0.62
416	203.1916	C10(13C)2H24O2	C12H24O2	-0.20
417	202.1881	C11(13C)1H24O2	C12H24O2	-1.03
418	75.0988	C1(13C)4H10	C5H10	-1.44
419	78.0906	C1(13C)3H10O	C4H10O	1.05
420	96.1011	C1(13C)3H12O2	C4H12O2	0.32
421	95.0976	C2(13C)2H12O2	C4H12O2	-1.44
422	77.0871	C2(13C)2H10O	C4H10O	-1.12
423	93.0910	C4H12O2	C4H12O2	-0.22
424	94.0945	C3(13C)1H12O2	C4H12O2	1.57
425	76.0840	C3(13C)1H10O	C4H10O	2.62
426	75.0805	C4H10O	C4H10O	0.41

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427	109.1133	C3(13C)2H14O2	C5H14O2	-0.85
428	108.1102	C4(13C)1H14O2	C5H14O2	1.77
429	107.1067	C5H14O2	C5H14O2	0.23
430	62.0683	C2(13C)1H8O	C3H8O	2.50
431	61.0648	C3H8O	C3H8O	-0.22
432	61.0478	C1(13C)1H5NO	C2H5NO	0.15
433	371.1017	C20(13C)3H13NO4	C23H13NO4	-0.28
434	194.0448	C9H7NO4	C9H7NO4	-0.17
435	90.0907	C2(13C)3H10O	C5H10O	2.48
436	72.0802	C2(13C)3H8	C5H8	3.82
437	71.0767	C3(13C)2H8	C5H8	1.50
438	70.0732	C4(13C)1H8	C5H8	-0.88
439	237.0394	C11H8O6	C11H8O6	-0.04
440	60.0810	C3H9N	C3H9N	3.27
441	229.0345	C9H8O7	C9H8O7	0.89
442	123.0716	C6(13C)2H8O	C8H8O	1.01
443	170.1256	C9(13C)1H16O2	C10H16O2	-0.60
444	103.0751	C5H10O2	C5H10O2	-2.27
445	106.0852	C2(13C)3H10O2	C5H10O2	-1.73
446	105.0822	C3(13C)2H10O2	C5H10O2	0.96
447	104.0786	C4(13C)1H10O2	C5H10O2	-0.64
448	77.0508	C1(13C)2H6O2	C3H6O2	0.16
449	134.1166	C4(13C)3H14O2	C7H14O2	-0.71
450	133.1136	C5(13C)2H14O2	C7H14O2	1.42
451	132.1100	C6(13C)1H14O2	C7H14O2	0.17
452	118.0581	C4(13C)1H8O3	C5H8O3	0.65
453	120.1009	C3(13C)3H12O2	C6H12O2	-1.16
454	119.0979	C4(13C)2H12O2	C6H12O2	1.22
455	118.0943	C5(13C)1H12O2	C6H12O2	-0.19
456	117.0456	C3(13C)2H6O3	C5H6O3	-0.95
457	119.0616	C3(13C)2H8O3	C5H8O3	2.05

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458	87.0717	C3(13C)2H8O	C5H8O	1.75
459	86.0681	C4(13C)1H8O	C5H8O	-0.18
460	190.1431	C7(13C)3H18O3	C10H18O3	0.95
461	189.1396	C8(13C)2H18O3	C10H18O3	0.07
462	188.1361	C9(13C)1H18O3	C10H18O3	-0.82
463	158.1442	C5(13C)5H16O	C10H16O	0.44
464	176.1547	C5(13C)5H18O2	C10H18O2	0.10
465	175.1512	C6(13C)4H18O2	C10H18O2	-0.85
466	157.1407	C6(13C)4H16O	C10H16O	-0.62
467	156.1376	C7(13C)3H16O	C10H16O	1.19
468	172.1411	C9(13C)1H18O2	C10H18O2	-1.16
469	171.1291	C8(13C)2H16O2	C10H16O2	0.38
470	173.1446	C8(13C)2H18O2	C10H18O2	-0.19
471	174.1482	C7(13C)3H18O2	C10H18O2	0.77
472	155.1341	C8(13C)2H16O	C10H16O	0.12
473	59.0403	C1(13C)2H4O	C3H4O	1.08
474	211.1973	C5(13C)10H20	C15H20	0.08
475	192.1587	C7(13C)3H20O3	C10H20O3	0.44
476	191.1556	C8(13C)2H20O3	C10H20O3	1.92
477	137.0999	C4(13C)1H13NO3	C5H13NO3	-2.30
478	122.0802	C2(13C)3H10O3	C5H10O3	-1.13
479	104.0697	C2(13C)3H8O2	C5H8O2	-0.83
480	101.0596	C5H8O2	C5H8O2	-1.36
481	119.0701	C5H10O3	C5H10O3	-1.58
482	120.0736	C4(13C)1H10O3	C5H10O3	-0.17
483	121.0771	C3(13C)2H10O3	C5H10O3	1.21
484	103.0666	C3(13C)2H8O2	C5H8O2	1.92
485	102.0631	C4(13C)1H8O2	C5H8O2	0.30
486	78.0633	C2(13C)1H8O2	C3H8O2	2.57
487	212.2004	C11(13C)3H24O	C14H24O	1.71
488	232.2175	C9(13C)5H26O2	C14H26O2	0.84

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489	204.1852	C7(13C)5H22O2	C12H22O2	-3.89
490	230.2109	C11(13C)3H26O2	C14H26O2	1.35
491	229.2074	C12(13C)2H26O2	C14H26O2	0.63
492	202.1795	C9(13C)3H22O2	C12H22O2	1.10
493	201.1760	C10(13C)2H22O2	C12H22O2	0.28
494	132.1011	C4(13C)3H12O2	C7H12O2	0.02
495	93.0820	C2(13C)2H10O2	C4H10O2	-0.43
496	92.0790	C3(13C)1H10O2	C4H10O2	2.66
497	91.0754	C4H10O2	C4H10O2	0.84
498	89.0872	C3(13C)2H10O	C5H10O	0.62
499	88.0837	C4(13C)1H10O	C5H10O	-1.28
500	77.0597	C3H8O2	C3H8O2	0.42
501	60.0527	C2(13C)1H6O	C3H6O	4.21
502	107.0977	C3(13C)2H12O2	C5H12O2	0.04
503	106.0942	C4(13C)1H12O2	C5H12O2	-1.54
504	105.0911	C5H12O2	C5H12O2	1.15
505	230.0380	C7(13C)4H3N3O3	C11H3N3O3	-0.59
506	75.0715	C2(13C)2H8O	C4H8O	0.15
507	74.0680	C3(13C)1H8O	C4H8O	-2.12
508	57.0610	C2(13C)2H6	C4H6	1.10
509	56.0575	C3(13C)1H6	C4H6	-1.90
510	160.1325	C6(13C)3H16O2	C9H16O2	0.57
511	159.1289	C7(13C)2H16O2	C9H16O2	-0.48
512	143.1340	C7(13C)2H16O	C9H16O	-0.85
513	153.1186	C8(13C)2H14O	C10H14O	0.75
514	117.0819	C4(13C)2H10O2	C6H10O2	-1.79
515	185.1721	C8(13C)4H20O	C12H20O	-0.05
516	184.1690	C9(13C)3H20O	C12H20O	1.49
517	183.1655	C10(13C)2H20O	C12H20O	0.58
518	130.0945	C6(13C)1H12O2	C7H12O2	0.91
519	131.0976	C5(13C)2H12O2	C7H12O2	-1.26

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520	116.0788	C5(13C)1H10O2	C6H10O2	0.64
521	186.1756	C7(13C)5H20O	C12H20O	0.85
522	163.1238	C6(13C)2H16O3	C8H16O3	-1.05
523	149.1081	C5(13C)2H14O3	C7H14O3	-1.45
524	148.1050	C6(13C)1H14O3	C7H14O3	0.46
525	213.2035	C10(13C)4H24O	C14H24O	0.37
526	135.0928	C4(13C)2H12O3	C6H12O3	1.41
527	134.0893	C5(13C)1H12O3	C6H12O3	0.18
528	107.0897	C3(13C)1H11NO2	C4H11NO2	0.43
529	158.1254	C8(13C)1H16O2	C9H16O2	-1.54
530	76.0473	C2(13C)1H6O2	C3H6O2	-2.05
531	89.0599	C4H8O2	C4H8O2	1.96
532	92.0700	C1(13C)3H8O2	C4H8O2	2.44
533	91.0665	C2(13C)2H8O2	C4H8O2	0.62
534	90.0630	C3(13C)1H8O2	C4H8O2	-1.23
535	73.0560	C2(13C)2H6O	C4H6O	1.48
536	72.0524	C3(13C)1H6O	C4H6O	-0.83
537	141.1104	C7(13C)1H13NO	C8H13NO	0.12
538	107.0767	C6(13C)2H8	C8H8	0.73
539	106.0731	C7(13C)1H8	C8H8	-0.84
540	62.0347	H3N3O	H3N3O	-3.10
541	108.0735	C3(13C)1H10O3	C4H10O3	-1.50
542	63.0351	(13C)2H4O2	C2H4O2	-0.51
543	62.0320	C1(13C)1H4O2	C2H4O2	4.10
544	61.0285	C2H4O2	C2H4O2	1.40
545	105.0611	C6(13C)2H6	C8H6	1.67
546	164.1273	C5(13C)3H16O3	C8H16O3	-0.03
547	150.1116	C4(13C)3H14O3	C7H14O3	-0.33
548	145.1410	C5(13C)4H16O	C9H16O	1.46
549	142.1139	C6(13C)2H13NO	C8H13NO	1.29
550	104.0576	C7(13C)1H6	C8H6	0.07

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551	188.1643	C8(13C)3H20O2	C11H20O2	3.34
552	109.0765	C2(13C)2H10O3	C4H10O3	-4.09
553	71.0494	C4H6O	C4H6O	3.18
554	162.1207	C7(13C)1H16O3	C8H16O3	0.69
555	152.1150	C9(13C)1H14O	C10H14O	-0.34
556	105.0701	C8H8	C8H8	1.86
557	182.1620	C11(13C)1H20O	C12H20O	-0.33
558	56.0212	C2(13C)1H2O	C3H2O	-0.13
559	262.2560	C9(13C)7H30O2	C16H30O2	2.35
560	288.2803	C13(13C)5H34O2	C18H34O2	1.29
561	242.2384	C11(13C)5H28O	C16H28O	1.38
562	258.2419	C13(13C)3H30O2	C16H30O2	-0.20
563	257.2388	C14(13C)2H30O2	C16H30O2	0.90
564	241.2349	C12(13C)4H28O	C16H28O	0.69
565	260.2489	C11(13C)5H30O2	C16H30O2	1.09
566	259.2463	C5(13C)12H26O	C17H26O	1.50
567	261.2529	C3(13C)14H26O	C17H26O	1.04
568	256.2263	C13(13C)3H28O2	C16H28O2	0.18
569	255.2237	C7(13C)10H24O	C17H24O	0.59
570	187.1603	C9(13C)2H20O2	C11H20O2	0.06
571	216.1952	C10(13C)3H24O2	C13H24O2	1.24
572	201.2038	C9(13C)4H24O	C13H24O	1.93
573	239.2193	C12(13C)4H26O	C16H26O	1.10
574	262.2918	C10(13C)7H34O	C17H34O	0.26
575	257.2746	C15(13C)2H34O	C17H34O	-1.22
576	202.2069	C8(13C)5H24O	C13H24O	0.52
577	199.1972	C4(13C)10H20	C14H20	-0.62
578	197.1996	C8(13C)6H22	C14H22	0.07
579	198.2031	C7(13C)7H22	C14H22	0.91
580	203.2104	C7(13C)6H24O	C13H24O	1.34
581	182.1898	C10(13C)3H22	C13H22	1.50

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582	183.1928	C9(13C)4H22	C13H22	-0.06
583	215.1917	C11(13C)2H24O2	C13H24O2	0.47
584	171.1654	C9(13C)2H20O	C11H20O	-0.20
585	214.2070	C9(13C)5H24O	C14H24O	1.15
586	241.2071	C13(13C)2H26O2	C15H26O2	-0.68
587	193.1864	C12(13C)2H22	C14H22	1.28
588	117.0371	C1(13C)4H4O3	C5H4O3	2.74
589	177.1395	C7(13C)2H18O3	C9H18O3	-0.72
590	178.1430	C6(13C)3H18O3	C9H18O3	0.22
591	176.1364	C8(13C)1H18O3	C9H18O3	0.89
592	108.0932	C2(13C)2H11NO2	C4H11NO2	1.98
593	245.2118	C7(13C)8H24O2	C15H24O2	0.13
594	244.2168	C10(13C)5H26O2	C15H26O2	-2.31
595	126.1359	C8(13C)1H16	C9H16	0.92
596	84.0889	C5(13C)1H10	C6H10	-0.20
597	228.2402	C14(13C)1H30O	C15H30O	-0.53
598	98.1046	C6(13C)1H12	C7H12	0.28
599	58.0367	C2(13C)1H4O	C3H4O	-1.81
600	260.2762	C10(13C)7H32O	C17H32O	0.63
601	246.2328	C10(13C)5H28O2	C15H28O2	-0.86
602	243.2231	C13(13C)2H28O2	C15H28O2	0.77
603	177.1946	C5(13C)6H22O	C11H22O	0.49
604	260.2852	C12(13C)5H34O	C17H34O	0.71
605	259.2817	C13(13C)4H34O	C17H34O	0.07
606	261.2887	C11(13C)6H34O	C17H34O	1.35
607	258.2782	C14(13C)3H34O	C17H34O	-0.57
608	148.1596	C4(13C)5H18O	C9H18O	-1.14
609	147.1566	C5(13C)4H18O	C9H18O	0.78
610	146.1531	C6(13C)3H18O	C9H18O	-0.35
611	145.1495	C7(13C)2H18O	C9H18O	-1.51
612	87.1079	C4(13C)2H12	C6H12	0.62

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613	172.1778	C10(13C)1H22O	C11H22O	0.89
614	144.1465	C8(13C)1H18O	C9H18O	0.45
615	116.1151	C6(13C)1H14O	C7H14O	-0.20
616	204.2229	C8(13C)5H26O	C13H26O	2.25
617	203.2194	C9(13C)4H26O	C13H26O	1.44
618	202.2154	C10(13C)3H26O	C13H26O	-1.61
619	201.2123	C11(13C)2H26O	C13H26O	-0.21
620	255.2591	C15(13C)2H32O	C17H32O	-0.86
621	205.2259	C7(13C)6H26O	C13H26O	0.85
622	176.1915	C6(13C)5H22O	C11H22O	2.10
623	175.1880	C7(13C)4H22O	C11H22O	1.16
624	174.1844	C8(13C)3H22O	C11H22O	0.21
625	173.1809	C9(13C)2H22O	C11H22O	-0.75
626	259.2732	C11(13C)6H32O	C17H32O	1.73
627	258.2701	C12(13C)5H32O	C17H32O	2.83
628	234.2609	C8(13C)7H30O	C15H30O	1.84
629	119.1252	C3(13C)4H14O	C7H14O	0.23
630	118.1217	C4(13C)3H14O	C7H14O	-1.19
631	117.1186	C5(13C)2H14O	C7H14O	1.23
632	233.2569	C9(13C)6H30O	C15H30O	-0.80
633	229.2437	C13(13C)2H30O	C15H30O	0.20
634	232.2538	C10(13C)5H30O	C15H30O	0.42
635	231.2503	C11(13C)4H30O	C15H30O	-0.30
636	230.2472	C12(13C)3H30O	C15H30O	0.93

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Table S3. Compounds contributing to PC1 (*i.e.*, absolute value loading > 0.01)

#	<i>m/z</i>	molecular formula (¹² C & ¹³ C)	Unique molecular formula	ID	Loading value
1	159.0653241	C7H10O4	C7H10O4		-0.02
2	145.1132461	C6(13C)2H14O2	C8H14O2		0.01
3	178.1703032	C5(13C)5H20O2	C10H20O2	Ethyl octanoate	0.01
3	177.1667822	C6(13C)4H20O2	C10H20O2	Ethyl octanoate	0.06
3	176.1637092	C7(13C)3H20O2	C10H20O2	Ethyl octanoate	0.12
3	175.1606362	C8(13C)2H20O2	C10H20O2	Ethyl octanoate	0.13
3	174.1571152	C9(13C)1H20O2	C10H20O2	Ethyl octanoate	0.07
4	112.1112931	C5(13C)3H12	C8H12		0.01
4	111.1077721	C6(13C)2H12	C8H12		0.01
5	212.2187852	C8(13C)7H24	C15H24	Farnesene	0.03
5	211.2152642	C9(13C)6H24	C15H24	Farnesene	0.07
5	210.2121912	C10(13C)5H24	C15H24	Farnesene	0.11
5	208.2051492	C12(13C)3H24	C15H24	Farnesene	0.08
5	207.2016282	C13(13C)2H24	C15H24	Farnesene	0.04
5	209.2086702	C11(13C)4H24	C15H24	Farnesene	0.12
6	153.1458941	C7(13C)4H16	C11H16		0.02
6	152.1423731	C8(13C)3H16	C11H16		0.02
6	151.1393001	C9(13C)2H16	C11H16		0.02
7	124.1114331	C6(13C)3H12	C9H12		0.01
7	123.1079121	C7(13C)2H12	C9H12		0.01
8	96.08900509	C6(13C)1H10	C7H10		0.01
8	97.09207809	C5(13C)2H10	C7H10		0.01
9	82.07331107	C5(13C)1H8	C6H8		0.01
9	83.07683208	C4(13C)2H8	C6H8		0.01
10	74.0957671	C2(13C)3H10	C5H10		0.01

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10	73.09224609	C3(13C)2H10	C5H10		0.05
10	72.08872509	C4(13C)1H10	C5H10		0.05
11	148.1323211	C5(13C)3H16O2	C8H16O2	Octanoic Acid	0.03
11	147.1288001	C6(13C)2H16O2	C8H16O2	Octanoic Acid	0.04
11	146.1257271	C7(13C)1H16O2	C8H16O2	Octanoic Acid	0.03
12	205.1977222	C8(13C)4H24O2	C12H24O2	Ethyl decanoate	0.03
12	206.2012432	C7(13C)5H24O2	C12H24O2	Ethyl decanoate	0.01
12	204.1950972	C9(13C)3H24O2	C12H24O2	Ethyl decanoate	0.05
12	203.1915762	C10(13C)2H24O2	C12H24O2	Ethyl decanoate	0.04
12	202.1880552	C11(13C)1H24O2	C12H24O2	Ethyl decanoate	0.02
13	95.0975801	C2(13C)2H12O2	C4H12O2	Ethanol	0.39
13	93.09098609	C4H12O2	C4H12O2	Ethanol	0.37
13	94.09450709	C3(13C)1H12O2	C4H12O2	Ethanol	0.76
14	77.08706609	C2(13C)2H10O	C4H10O		0.07
14	76.08399308	C3(13C)1H10O	C4H10O		0.14
14	75.08047208	C4H10O	C4H10O		0.07
15	71.07669208	C3(13C)2H8	C5H8		0.01
15	70.07317107	C4(13C)1H8	C5H8		0.01
16	101.0595701	C5H8O2	C5H8O2		0.02
16	103.0666121	C3(13C)2H8O2	C5H8O2		0.03
16	102.0630911	C4(13C)1H8O2	C5H8O2		0.06
17	120.0736051	C4(13C)1H10O3	C5H10O3		0.01
18	90.06295106	C3(13C)1H8O2	C4H8O2		0.02
19	106.0731431	C7(13C)1H8	C8H8		-0.02
19	105.0700701	C8H8	C8H8		-0.01
20	62.03201103	C1(13C)1H4O2	C2H4O2	Acetic acid	-0.04
20	61.02849003	C2H4O2	C2H4O2	Acetic acid	-0.04

Table S4. Compounds contributing to PC2 (*i.e.*, absolute value loading > 0.01)

#	<i>m/z</i>	molecular formula (¹² C & ¹³ C)	Unique molecular formula	ID	Loading value
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1	227.0386	C9(13C)1H3N5O2	C10H3N5O2		0.13
1	226.0356	C10H3N5O2	C10H3N5O2		0.12
1	228.0422	C8(13C)2H3N5O2	C10H3N5O2		0.02
2	228.0314	C9(13C)2H3N3O3	C11H3N3O3		0.01
3	192.0480	C8(13C)1H6N2O3	C9H6N2O3		0.07
4	172.1326	C7(13C)3H16O2	C10H16O2	Geranic acid	0.03
4	170.1256	C9(13C)1H16O2	C10H16O2	Geranic acid	0.03
4	171.1291	C8(13C)2H16O2	C10H16O2	Geranic acid	0.05
5	102.0268	C3(13C)1H4O3	C4H4O3		0.01
6	192.1676	C9(13C)1H22O3	C10H22O3		0.02
6	191.1641	C10H22O3	C10H22O3		0.17
7	201.1120	C10H16O4	C10H16O4		0.02
8	160.0684	C6(13C)1H10O4	C7H10O4		0.03
8	159.0653	C7H10O4	C7H10O4		0.34
9	236.1129	C7(13C)3H16O6	C10H16O6		0.03
10	113.0508	C4(13C)2H6O2	C6H6O2		0.01
11	100.0475	C4(13C)1H6O2	C5H6O2		0.05
11	101.0506	C3(13C)2H6O2	C5H6O2		0.04
12	104.0424	C3(13C)1H6O3	C4H6O3		0.01
13	76.0392	C2H5NO2	C2H5NO2		0.02
14	188.1276	C7(13C)3H16O3	C10H16O3		0.04
14	187.1240	C8(13C)2H16O3	C10H16O3		0.04
14	186.1205	C9(13C)1H16O3	C10H16O3		0.02
15	169.1135	C8(13C)2H14O2	C10H14O2		0.01
16	144.0734	C6(13C)1H10O3	C7H10O3		0.03
16	145.0770	C5(13C)2H10O3	C7H10O3		0.03
17	131.0613	C4(13C)2H8O3	C6H8O3		0.03
17	130.0577	C5(13C)1H8O3	C6H8O3		0.04
18	114.0632	C5(13C)1H8O2	C6H8O2	Sorbic acid	0.06
18	115.0663	C4(13C)2H8O2	C6H8O2	Sorbic acid	0.05
19	89.0509	C2(13C)2H6O2	C4H6O2		0.01

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19	88.0474	C3(13C)1H6O2	C4H6O2	0.03
20	133.0768	C4(13C)2H10O3	C6H10O3	0.02
20	132.0737	C5(13C)1H10O3	C6H10O3	0.03
21	129.0820	C5(13C)2H10O2	C7H10O2	0.03
22	115.1026	C5(13C)2H12O	C7H12O	0.01
23	101.0873	C4(13C)2H10O	C6H10O	0.01
24	157.1134	C7(13C)2H14O2	C9H14O2	0.01
25	113.0870	C5(13C)2H10O	C7H10O	0.01
26	99.0713	C4(13C)2H8O	C6H8O	0.01
26	98.0683	C5(13C)1H8O	C6H8O	0.01
27	160.0962	C5(13C)3H12O3	C8H12O3	0.02
27	159.0927	C6(13C)2H12O3	C8H12O3	0.04
27	158.0891	C7(13C)1H12O3	C8H12O3	0.03
28	142.0942	C7(13C)1H12O2	C8H12O2	0.04
28	144.1012	C5(13C)3H12O2	C8H12O2	0.03
28	143.0977	C6(13C)2H12O2	C8H12O2	0.06
29	147.1198	C4(13C)4H14O2	C8H14O2	0.02
29	144.1102	C7(13C)1H14O2	C8H14O2	0.07
29	146.1168	C5(13C)3H14O2	C8H14O2	0.06
29	145.1132	C6(13C)2H14O2	C8H14O2	0.10
30	162.1117	C5(13C)3H14O3	C8H14O3	0.01
30	161.1082	C6(13C)2H14O3	C8H14O3	0.02
30	160.1051	C7(13C)1H14O3	C8H14O3	0.02
31	127.1027	C6(13C)2H12O	C8H12O	0.06
31	128.1058	C5(13C)3H12O	C8H12O	0.02
32	127.0664	C5(13C)2H8O2	C7H8O2	0.01
33	157.0771	C6(13C)2H10O3	C8H10O3	0.01
34	141.0821	C6(13C)2H10O2	C8H10O2	0.01
34	140.0786	C7(13C)1H10O2	C8H10O2	0.01
35	125.0872	C6(13C)2H10O	C8H10O	0.01
36	143.0614	C5(13C)2H8O3	C7H8O3	0.01

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36	142.0579	C6(13C)1H8O3	C7H8O3		0.01
37	116.0425	C4(13C)1H6O3	C5H6O3		0.04
37	117.0456	C3(13C)2H6O3	C5H6O3		0.01
38	178.1703	C5(13C)5H20O2	C10H20O2	Ethyl octanoate	0.01
38	177.1668	C6(13C)4H20O2	C10H20O2	Ethyl octanoate	0.06
38	176.1637	C7(13C)3H20O2	C10H20O2	Ethyl octanoate	0.16
38	175.1606	C8(13C)2H20O2	C10H20O2	Ethyl octanoate	0.20
38	174.1571	C9(13C)1H20O2	C10H20O2	Ethyl octanoate	0.12
39	126.1270	C6(13C)3H14	C9H14		0.01
39	125.1235	C7(13C)2H14	C9H14		0.01
40	112.1113	C5(13C)3H12	C8H12		0.01
40	111.1078	C6(13C)2H12	C8H12		0.01
41	212.2188	C8(13C)7H24	C15H24	Farnesene	0.01
41	211.2153	C9(13C)6H24	C15H24	Farnesene	0.04
41	210.2122	C10(13C)5H24	C15H24	Farnesene	0.08
41	208.2051	C12(13C)3H24	C15H24	Farnesene	0.09
41	207.2016	C13(13C)2H24	C15H24	Farnesene	0.04
41	209.2087	C11(13C)4H24	C15H24	Farnesene	0.11
42	124.1114	C6(13C)3H12	C9H12		0.01
42	123.1079	C7(13C)2H12	C9H12		0.01
43	152.1424	C8(13C)3H16	C11H16		0.02
43	151.1393	C9(13C)2H16	C11H16		0.01
44	96.0890	C6(13C)1H10	C7H10		0.01
44	98.0956	C4(13C)3H10	C7H10		0.01
44	97.0921	C5(13C)2H10	C7H10		0.02
45	74.0958	C2(13C)3H10	C5H10		0.03
45	73.0922	C3(13C)2H10	C5H10		0.13
45	72.0887	C4(13C)1H10	C5H10		0.15
46	149.1354	C4(13C)4H16O2	C8H16O2	Octanoic acid	0.01
46	148.1323	C5(13C)3H16O2	C8H16O2	Octanoic acid	0.07
46	147.1288	C6(13C)2H16O2	C8H16O2	Octanoic acid	0.13

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46	146.1257	C7(13C)1H16O2	C8H16O2	Octanoic acid	0.11
46	145.1222	C8H16O2	C8H16O2	Octanoic acid	0.03
47	139.1302	C6(13C)4H14	C10H14		0.01
47	138.1267	C7(13C)3H14	C10H14		0.02
47	137.1236	C8(13C)2H14	C10H14		0.02
48	83.0768	C4(13C)2H8	C6H8		0.02
49	140.1427	C7(13C)3H16	C10H16		0.01
50	108.0887	C7(13C)1H10	C8H10		-0.02
51	59.0766	C2(13C)2H8	C4H8		0.01
51	58.0735	C3(13C)1H8	C4H8		0.02
52	229.2347	C11(13C)4H28O	C15H28O		-0.01
53	204.1951	C9(13C)3H24O2	C12H24O2	Ethyl decanoate	0.04
53	203.1916	C10(13C)2H24O2	C12H24O2	Ethyl decanoate	0.04
53	202.1881	C11(13C)1H24O2	C12H24O2	Ethyl decanoate	0.01
54	95.0976	C2(13C)2H12O2	C4H12O2		-0.14
54	94.0945	C3(13C)1H12O2	C4H12O2		-0.14
55	77.0871	C2(13C)2H10O	C4H10O		-0.02
55	76.0840	C3(13C)1H10O	C4H10O		-0.02
56	371.1017	C20(13C)3H13NO4	C23H13NO4		0.01
57	229.0345	C9H8O7	C9H8O7		0.01
58	103.0751	C5H10O2	C5H10O2		0.03
58	105.0822	C3(13C)2H10O2	C5H10O2		0.04
58	104.0786	C4(13C)1H10O2	C5H10O2		0.07
59	133.1136	C5(13C)2H14O2	C7H14O2		0.01
60	118.0581	C4(13C)1H8O3	C5H8O3		0.01
61	120.1009	C3(13C)3H12O2	C6H12O2	Hexanoic acid	0.01
61	119.0979	C4(13C)2H12O2	C6H12O2	Hexanoic acid	0.04
61	118.0943	C5(13C)1H12O2	C6H12O2	Hexanoic acid	0.05
62	87.0717	C3(13C)2H8O	C5H8O		0.02
62	86.0681	C4(13C)1H8O	C5H8O		0.03
63	190.1431	C7(13C)3H18O3	C10H18O3		0.02

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63	189.1396	C8(13C)2H18O3	C10H18O3		0.02
63	188.1361	C9(13C)1H18O3	C10H18O3		0.01
64	176.1547	C5(13C)5H18O2	C10H18O2		0.01
64	175.1512	C6(13C)4H18O2	C10H18O2		0.05
64	172.1411	C9(13C)1H18O2	C10H18O2		0.06
64	173.1446	C8(13C)2H18O2	C10H18O2		0.12
64	174.1482	C7(13C)3H18O2	C10H18O2		0.11
65	157.1407	C6(13C)4H16O	C10H16O	Citral	0.03
65	156.1376	C7(13C)3H16O	C10H16O	Citral	0.07
65	155.1341	C8(13C)2H16O	C10H16O	Citral	0.08
66	104.0697	C2(13C)3H8O2	C5H8O2		0.02
66	101.0596	C5H8O2	C5H8O2		0.20
66	103.0666	C3(13C)2H8O2	C5H8O2		0.22
66	102.0631	C4(13C)1H8O2	C5H8O2		0.47
67	120.0736	C4(13C)1H10O3	C5H10O3		0.06
67	121.0771	C3(13C)2H10O3	C5H10O3		0.05
68	202.1795	C9(13C)3H22O2	C12H22O2		0.02
68	201.1760	C10(13C)2H22O2	C12H22O2		0.01
69	77.0597	C3H8O2	C3H8O2		-0.02
70	74.0680	C3(13C)1H8O	C4H8O		0.01
71	160.1325	C6(13C)3H16O2	C9H16O2		0.01
71	159.1289	C7(13C)2H16O2	C9H16O2		0.01
72	153.1186	C8(13C)2H14O	C10H14O		0.02
73	117.0819	C4(13C)2H10O2	C6H10O2		0.03
73	116.0788	C5(13C)1H10O2	C6H10O2		0.03
74	130.0945	C6(13C)1H12O2	C7H12O2		0.01
74	131.0976	C5(13C)2H12O2	C7H12O2		0.02
75	89.0599	C4H8O2	C4H8O2		0.09
75	91.0665	C2(13C)2H8O2	C4H8O2		0.06
75	90.0630	C3(13C)1H8O2	C4H8O2		0.19
76	73.0560	C2(13C)2H6O	C4H6O		0.01

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76	72.0524	C3(13C)1H6O	C4H6O	0.03
77	107.0767	C6(13C)2H8	C8H8	0.12
77	106.0731	C7(13C)1H8	C8H8	0.21
77	105.0701	C8H8	C8H8	0.09
78	62.0320	C1(13C)1H4O2	C2H4O2	-0.02
78	61.0285	C2H4O2	C2H4O2	0.04
79	84.0889	C5(13C)1H10	C6H10	-0.02
80	98.1046	C6(13C)1H12	C7H12	-0.01
81	58.0367	C2(13C)1H4O	C3H4O	-0.01
82	147.1566	C5(13C)4H18O	C9H18O	-0.01
82	146.1531	C6(13C)3H18O	C9H18O	-0.02
82	145.1495	C7(13C)2H18O	C9H18O	-0.02
82	144.1465	C8(13C)1H18O	C9H18O	-0.02
83	172.1778	C10(13C)1H22O	C11H22O	-0.01
83	175.1880	C7(13C)4H22O	C11H22O	-0.02
83	174.1844	C8(13C)3H22O	C11H22O	-0.02
83	173.1809	C9(13C)2H22O	C11H22O	-0.02
84	203.2194	C9(13C)4H26O	C13H26O	-0.02
84	202.2154	C10(13C)3H26O	C13H26O	-0.02
85	118.1217	C4(13C)3H14O	C7H14O	-0.02
85	117.1186	C5(13C)2H14O	C7H14O	-0.02
86	233.2569	C9(13C)6H30O	C15H30O	-0.01
86	229.2437	C13(13C)2H30O	C15H30O	-0.01
86	232.2538	C10(13C)5H30O	C15H30O	-0.03
86	231.2503	C11(13C)4H30O	C15H30O	-0.03
86	230.2472	C12(13C)3H30O	C15H30O	-0.03

Table S5. Compounds detected in negative ion mode during yeast growth in $^{13}\text{C}_1$ -glucose. All the analytes were detected in $[\text{M}-\text{H}]^-$ form.

#	m/z	molecular formula (^{12}C & ^{13}C)	Unique molecular formula	RDBE	Mass error (ppm)	ID
1	58.03793	C2(13C)1H6O	C3H6O	1	-0.23	

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2	59.01383	C2H4O2	C2H4O2	1	-0.38	Acetic acid
2	60.0172	C1(13C)1H4O2	C2H4O2	1	-0.13	Acetic acid
2	61.02057	(13C)2H4O2	C2H4O2	1	0.11	Acetic acid
3	73.02951	C3H6O2	C3H6O2	1	0.09	Propionic acid
3	74.03288	C2(13C)1H6O2	C3H6O2	1	0.29	Propionic acid
4	86.0693	C4(13C)1H10O	C5H10O	1	0.65	
4	87.07252	C3(13C)2H10O	C5H10O	1	-0.89	
5	87.0452	C4H8O2	C4H8O2	1	0.53	Butanoic acid
5	88.04857	C3(13C)1H8O2	C4H8O2	1	0.70	Butanoic acid
5	89.05194	C2(13C)2H8O2	C4H8O2	1	0.85	Butanoic acid
5	90.05516	C1(13C)3H8O2	C4H8O2	1	-0.64	Butanoic acid
6	104.0708	C2(13C)3H10O2	C5H10O2	1	-0.65	Pentanoic acid
7	113.0973	C7H14O	C7H14O	1	0.98	Heptanoic acid
7	114.1005	C6(13C)1H14O	C7H14O	1	-0.38	Heptanoic acid
7	115.1039	C5(13C)2H14O	C7H14O	1	0.01	Heptanoic acid
7	116.1073	C4(13C)3H14O	C7H14O	1	0.40	Heptanoic acid
8	115.0766	C6H12O2	C6H12O2	1	1.26	Hexanoic acid
8	116.0799	C5(13C)1H12O2	C6H12O2	1	0.78	Hexanoic acid
8	117.0832	C4(13C)2H12O2	C6H12O2	1	0.31	Hexanoic acid
8	118.0865	C3(13C)3H12O2	C6H12O2	1	-0.15	Hexanoic acid
9	119.0349	C4H8O4	C4H8O4	1	-0.69	
9	120.0383	C3(13C)1H8O4	C4H8O4	1	-0.31	
9	121.0417	C2(13C)2H8O4	C4H8O4	1	0.06	
10	134.054	C4(13C)1H10O4	C5H10O4	1	0.09	
10	135.0574	C3(13C)2H10O4	C5H10O4	1	0.42	
11	142.1317	C8(13C)1H18O	C9H18O	1	-1.00	
11	143.1354	C7(13C)2H18O	C9H18O	1	1.40	
11	144.1388	C6(13C)3H18O	C9H18O	1	1.70	
11	145.1426	C5(13C)4H18O	C9H18O	1	4.73	
12	143.1076	C8H16O2	C8H16O2	1	-1.06	Octanoic acid
12	144.1112	C7(13C)1H16O2	C8H16O2	1	0.63	Octanoic acid

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12	145.1144	C6(13C)2H16O2	C8H16O2	1	-0.43	Octanoic acid
12	146.1179	C5(13C)3H16O2	C8H16O2	1	0.56	Octanoic acid
12	147.1211	C4(13C)4H16O2	C8H16O2	1	-0.50	Octanoic acid
12	148.1243	C3(13C)5H16O2	C8H16O2	1	-1.53	Octanoic acid
13	147.0665	C6H12O4	C6H12O4	1	1.47	
13	148.0695	C5(13C)1H12O4	C6H12O4	1	-0.92	
14	162.0854	C6(13C)1H14O4	C7H14O4	1	0.69	
15	172.1427	C9(13C)1H20O2	C10H20O2	1	1.68	Decanoic acid
15	173.1459	C8(13C)2H20O2	C10H20O2	1	0.78	Decanoic acid
15	174.149	C7(13C)3H20O2	C10H20O2	1	-0.68	Decanoic acid
15	175.1522	C6(13C)4H20O2	C10H20O2	1	-1.55	Decanoic acid
15	176.1556	C5(13C)5H20O2	C10H20O2	1	-1.29	Decanoic acid
16	175.0971	C8H16O4	C8H16O4	1	-2.74	
16	176.1006	C7(13C)1H16O4	C8H16O4	1	-1.91	
16	177.1043	C6(13C)2H16O4	C8H16O4	1	0.04	
17	188.1373	C9(13C)1H20O3	C10H20O3	1	-0.12	
17	189.1408	C8(13C)2H20O3	C10H20O3	1	0.64	
17	190.1441	C7(13C)3H20O3	C10H20O3	1	0.35	
17	191.1474	C6(13C)4H20O3	C10H20O3	1	0.06	
18	189.1134	C9H18O4	C9H18O4	1	0.88	
18	190.1164	C8(13C)1H18O4	C9H18O4	1	-0.98	
18	191.1203	C7(13C)2H18O4	C9H18O4	1	1.86	
18	192.1233	C6(13C)3H18O4	C9H18O4	1	0.01	
18	193.1266	C5(13C)4H18O4	C9H18O4	1	-0.27	
19	200.1734	C11(13C)1H24O2	C12H24O2	1	-1.53	Dodecanoic acid
19	201.1773	C10(13C)2H24O2	C12H24O2	1	1.17	Dodecanoic acid
19	202.1803	C9(13C)3H24O2	C12H24O2	1	-0.58	Dodecanoic acid
19	203.184	C8(13C)4H24O2	C12H24O2	1	1.11	Dodecanoic acid
19	204.1868	C7(13C)5H24O2	C12H24O2	1	-1.60	Dodecanoic acid
19	205.1908	C6(13C)6H24O2	C12H24O2	1	1.53	Dodecanoic acid
20	206.1392	C7(13C)3H20O4	C10H20O4	1	1.22	

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21	218.1477	C10(13C)1H22O4	C11H22O4	1	-0.86	
21	219.1513	C9(13C)2H22O4	C11H22O4	1	0.26	
21	220.1547	C8(13C)3H22O4	C11H22O4	1	0.46	
22	229.2086	C12(13C)2H28O2	C14H28O2	1	1.03	Tetradecanoic acid
22	230.212	C11(13C)3H28O2	C14H28O2	1	1.22	Tetradecanoic acid
22	232.2186	C9(13C)5H28O2	C14H28O2	1	0.73	Tetradecanoic acid
23	234.1693	C9(13C)3H24O4	C12H24O4	1	-4.03	
24	246.1795	C12(13C)1H26O4	C13H26O4	1	1.26	Tridecanoic acid
24	247.1828	C11(13C)2H26O4	C13H26O4	1	1.04	Tridecanoic acid
24	248.1861	C10(13C)3H26O4	C13H26O4	1	0.81	Tridecanoic acid
24	249.189	C9(13C)4H26O4	C13H26O4	1	-1.01	Tridecanoic acid
25	101.0519	C3(13C)2H8O2	C5H8O2	2	0.36	
26	103.0312	C2(13C)2H6O3	C4H6O3	2	0.70	
27	114.0641	C5(13C)1H10O2	C6H10O2	2	-0.51	
28	119.026	C2(13C)2H6O4	C4H6O4	2	-0.35	
29	131.0624	C4(13C)2H10O3	C6H10O3	2	-0.21	
29	132.0656	C3(13C)3H10O3	C6H10O3	2	-1.37	
30	142.0956	C7(13C)1H14O2	C8H14O2	2	0.99	
30	143.0991	C6(13C)2H14O2	C8H14O2	2	1.99	
30	144.1022	C5(13C)3H14O2	C8H14O2	2	0.22	
31	145.0781	C5(13C)2H12O3	C7H12O3	2	0.15	
31	146.0818	C4(13C)3H12O3	C7H12O3	2	2.50	
32	158.0904	C7(13C)1H14O3	C8H14O3	2	0.17	
32	159.0938	C6(13C)2H14O3	C8H14O3	2	0.45	
32	160.0968	C5(13C)3H14O3	C8H14O3	2	-1.76	
32	161.1005	C4(13C)4H14O3	C8H14O3	2	0.38	
33	169.1236	C10H18O2	C10H18O2	2	1.16	
33	170.1268	C9(13C)1H18O2	C10H18O2	2	0.24	
33	171.1303	C8(13C)2H18O2	C10H18O2	2	1.08	
33	172.1334	C7(13C)3H18O2	C10H18O2	2	-0.40	
33	173.1374	C6(13C)4H18O2	C10H18O2	2	3.31	

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34	175.0887	C6(13C)2H14O4	C8H14O4	2	0.33
34	176.0919	C5(13C)3H14O4	C8H14O4	2	-0.55
35	186.1218	C9(13C)1H18O3	C10H18O3	2	0.68
35	187.1251	C8(13C)2H18O3	C10H18O3	2	0.38
35	188.1282	C7(13C)3H18O3	C10H18O3	2	-0.97
35	189.132	C6(13C)4H18O3	C10H18O3	2	1.38
36	216.1596	C9(13C)3H22O3	C12H22O3	2	-0.38
36	217.1628	C8(13C)4H22O3	C12H22O3	2	-1.09
37	221.067	C8H14O7	C8H14O7	2	1.46
37	222.0699	C7(13C)1H14O7	C8H14O7	2	-0.59
38	177.1088	(13C)6H12N4O2	C6H12N4O2	3	-0.44
39	206.1426	C1(13C)7H16N4O2	C8H16N4O2	3	-4.51
39	207.1466	(13C)8H16N4O2	C8H16N4O2	3	-1.39
40	174.0897	C1(13C)5H10N4O2	C6H10N4O2	4	-0.99
41	203.125	C2(13C)6H14N4O2	C8H14N4O2	4	2.31
41	204.1281	C1(13C)7H14N4O2	C8H14N4O2	4	1.05
41	205.1312	(13C)8H14N4O2	C8H14N4O2	4	-0.19
42	231.2154	C3(13C)12H24O	C15H24O	4	-1.29
43	215.1567	C3(13C)10H18O2	C13H18O2	5	-1.17