

Electronic Supplementary Information

Table S1. Calculated retention indices for all identified compounds.

Compound Name	RT (min)	RI calc	RI NIST
Acetals			
acetal	5.686	889	NA
2,4,5-trimethyl-1,3-dioxolane	7.388	981	994
Alcohols			
2-methyl-1-propanol	10.326	1087	1092
3-methyl-1-butanol	13.891	1202	1209
3-methyl-3-buten-1-ol	15.153	1242	1248
1-pentanol	15.196	1244	1250
3-pentanol	17.996	1338	NA
1-hexanol	18.229	1346	1355
3-ethoxy-1-propanol	18.895	1369	1373
2-methyl-1-butanol	20.115	1413	NA
Aldehydes			
2-methyl-butanal	6.106	918	914
3-methyl-butanal	6.168	922	918
pentanal	7.457	984	979
hexanal	10.034	1077	1083
Aromatic compounds			
1,3-di-tert-butylbenzene	20.334	1421	1420
tetramethyl-pyrazine	21.853	1478	NA
ethyl phenylacetate	29.126	1779	1783
benzyl alcohol	31.091	1869	1870
phenylethyl alcohol	31.897	1907	1906
Carboxylic acids			
diethyl-acetic acid	18.842	1367	NA
acetic acid	20.647	1433	1449
propanoic acid	23.086	1525	1535
2-methyl-propanoic acid	23.729	1551	1570
2-methyl-butanoic acid	26.224	1653	1662
3-methyl-butanoic acid	26.264	1655	1666
hexanoic acid	30.228	1829	1846
Esters			
ethyl acetate	5.614	883	888
ethyl butyrate	8.739	1031	1035
ethyl 2-methylbutyrate	9.129	1045	1051
ethyl isovalerate	9.546	1060	1068
isoamyl acetate	11.218	1117	1122
ethyl hexanoate	14.665	1227	1233
ethyl lactate	17.796	1331	1347
Acetoin acetate	18.987	1373	1389
3-oxobutan-2-yl 2-methylbutanoate	22.784	1514	NA
Compound Name	RT (min)	RI calc	RI NIST
Esters			
ethyl 2-hydroxy-4-methylvalerate	23.256	1532	1547
ethyl myristate	34.642	2042	NA
ethyl palmitate	38.407	2246	2251
(e)-ethyl 9-octadecenoate	41.732	2473	NA
ethyl linoleate	42.466	2520	NA
Furans			
2-ethyl-furan	6.781	956	950
2-pentyl-furan	14.479	1221	1231
2-furanmethanol	26.040	1645	1660
Ketones			
2-butanone	5.905	905	907
2-heptanone	13.159	1179	1182
3-octanone	15.419	1251	1253
acetoin	17.340	1315	1284
2-hydroxy-3-pentanone	18.426	1353	1366
4-hydroxy-4-methyl-2-pentanone	18.635	1360	1358
2-nonanone	19.374	1386	1390
2,2-dimethyl-3-heptanone	20.466	1426	NA
Phenols			
mequinol	30.694	1851	NA
2-ethyl-phenol	36.872	2158	2157
2-methoxy-4-vinylphenol	37.400	2187	2188
Terpenoids			
caryophyllene	25.037	1604	1595

Table S2. Nutritional Information of unfermented oat substrate[†].

Nutritional component	Amount	Units	Method
Energy	1125	kJ/100g	(by calculation) FSANZ 1.2.8 ₁
Protein	15.7	%	AOAC 981.10 online (modified) ₂
Moisture	9.9	%	AOAC online 950.46B
Fat (total)	6.6	%	Acid Hydrolysis and Solvent Extraction ₃
Saturated Fat	1.5	%	AOAC 2012.13 modified
Ash	0.80%	%	AOAC online 942.05
Carbohydrates	46.9	%	(by difference) FSANZ 1.2.8
Total Sugars	0.6	%	Biopharm enzymatic ₄
Dietary Fiber	20.2	%	AOAC 991.43 online edition
Sodium	<0.5	mg/100g	ICP-MS

[†]Test results carried out by ICP-MS have been approved for release by ICP-MS KTP

₁ (CHO/energy by diff/calculation)

₂ Protein factor used 6.25

₃ Total fat extraction carried out after acid hydrolysis of the sample.

₄ Total sugars determined as individual mono- & disaccharides.

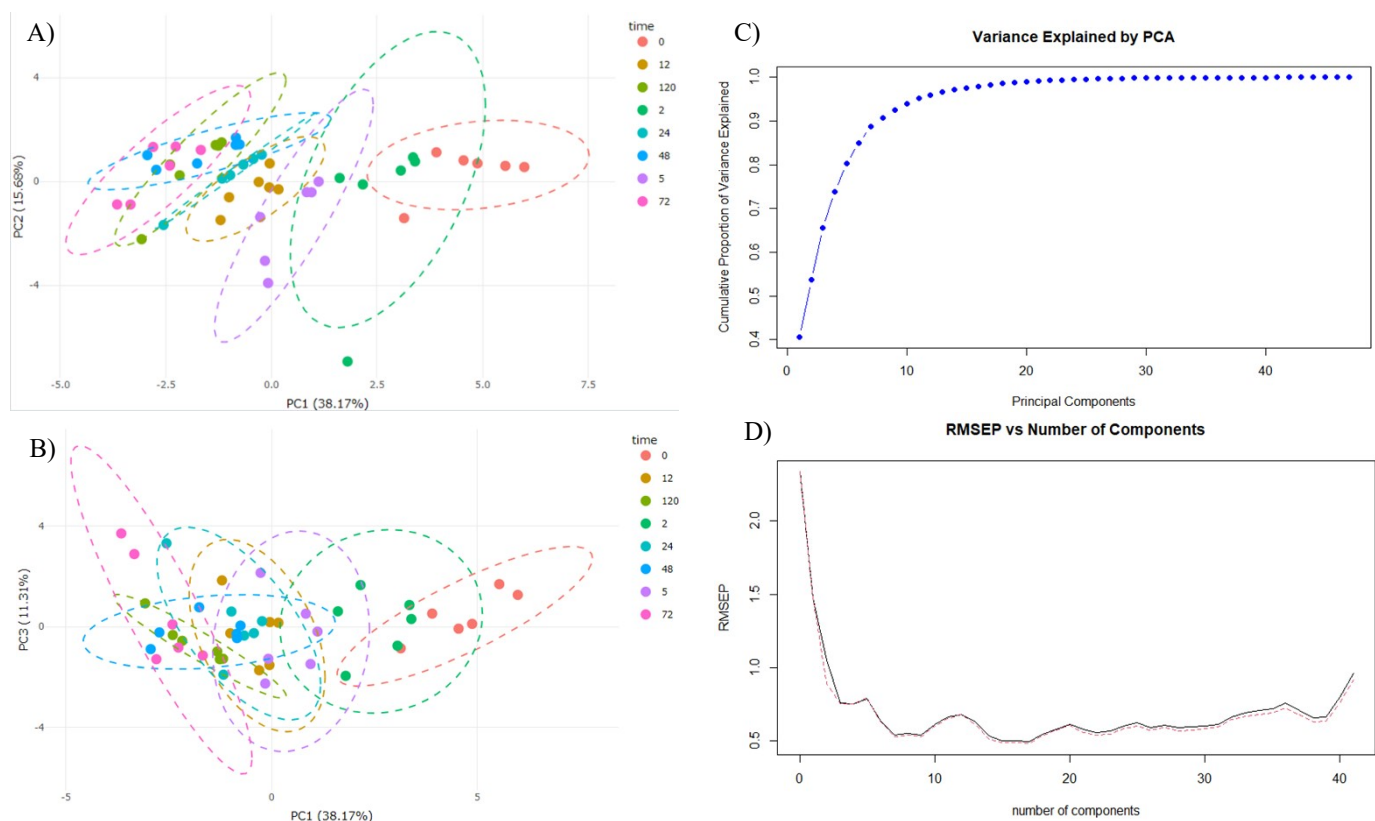


Figure S1. Principal Component Analysis of *Lactopantibacillus plantarum* solid-state fermented oat volatiles over 120 h. A) Principal components 1 and 2 scores plot indicating time point volatile separation, B) Principal components 1 and 3 scores plot indicating time point volatile separation, C) cumulative variance captured by increasing principal component number by the model, D) Root mean squared error of prediction decrease with increasing principal component number by the model.

Table S3. Pre-processed headspace solid-phase microextraction gas chromatography coupled to mass spectrometry peak area data.

Volatile	Timepoint							
	0	0	0	0	0	0	2	2
ethyl acetate	2820641	2188260	1835994	1717386	896322	1433815	1969079	1860595
acetal	18474	17424	13788	12486	494	10094	18400	19860
2-butanone	409901	362418	234844	225605	115931	182265	334259	288951
2-methyl-butanal	372881	311212	269497	251007	102700	204514	170880	141257
3-methyl-butanal	557331	461906	381193	357837	150349	297323	316567	257949
2-ethyl-furan	411481	310357	382494	319446	256165	299590	287423	224499
2,4,5-trimethyl-1,3-dioxolane	4523	3539	2317	4892	15008	1715	3502	3875
pentanal	1003329	842772	889424	787534	703794	601488	473999	336907
ethyl butyrate	32867	28880	21978	20640	26943	16777	25581	23539
ethyl 2-methylbutyrate	4963	6272	4135	3977	4134	3200	4106	4913
ethyl isovalerate	1545	1218	998	729	2360	1230	940	1433
hexanal	1175242	2034476	1115411	901505	1378546	1085871	351079	401687
2-methyl-1-propanol	41433	14062	30247	28919	38085	20768	26690	37332
isoamyl acetate	16130	17034	12972	12224	3556	12533	8593	12759
2-heptanone	69316	30715	101318	89790	87515	56863	47787	42847
3-methyl-1-butanol	76479	78637	70631	69021	61960	63933	100663	127187
2-pentyl-furan	919527	509483	1294966	1122748	209829	835749	592131	553123
ethyl hexanoate	1846	0	0	0	0	0	0	0
3-methyl-3-buten-1-ol	6681	7524	6399	6413	5090	6052	12521	12464
1-pentanol	389161	312990	340217	328336	332718	251134	477290	435293
3-octanone	7153	6821	6965	6173	3599	4428	5166	6327
acetoin	170347	127759	171837	146369	116148	145977	325123	712043
ethyl lactate	21313	25898	17493	16851	13730	15932	20637	31505
3-pentanol	9025	12111	9827	8806	11194	7624	10002	11916
1-hexanol	388085	334050	615272	567901	380000	461292	1009380	1043258
2-hydroxy-3-pentanone	10887	12801	9868	8830	4995	8072	12241	16968
4-hydroxy-4-methyl-2-pentanone	155269	93955	55759	133754	426486	72384	121760	106346
diethyl-acetic acid	1269	1832	951	605	1560	716	1942	2862
3-ethoxy-1-propanol	4314	5354	2893	2715	8028	3296	4445	7725
acetoin acetate	6019	6095	4869	5268	19730	4222	7464	8758
2-nonanone	3680	4331	3976	3719	5980	3119	3218	5253
2-methyl-1-butanol	9849	13763	10993	10374	23156	8268	6386	14007
1,3-di-tert-butylbenzene	41528	42264	47180	43083	60490	33694	40861	39638
2,2-dimethyl-3-heptanone	5748	6772	5483	4421	559	3156	4114	6952
acetic acid	151001	144218	210717	190440	250725	136397	162621	169976
tetramethyl-pyrazine	3872	7351	776	746	555	2411	3113	7247
3-oxobutan-2-yl 2-methylbutanoate	0	226	97	0	0	59	295	904
propanoic acid	675	1591	0	502	6248	1008	2579	6167
ethyl 2-hydroxy-4-methylvalerate	2116	2525	2374	2098	2112	2076	2832	3877
2-methyl-propanoic acid	5822	4883	14618	16737	180248	5347	8449	15230
caryophyllene	521	573	1213	1077	2204	618	408	802
2-furanmethanol	10616	9086	12153	10820	13164	8627	10447	11159
2-methyl-butanoic acid	12958	12666	19198	20257	131508	11892	21315	39610
3-methyl-butanoic acid	9322	8820	14524	15767	120085	10607	11523	19680
ethyl phenylacetate	635	558	611	437	521	3067	631	3960
hexanoic acid	44782	40352	33577	33418	40822	28608	50271	57153
mequinol	4362	4331	5029	4914	6574	3853	5179	5274
benzyl alcohol	765	775	3987	3763	4443	3087	1106	1701
phenylethyl alcohol	2785	3105	8534	8697	14911	38693	5720	56905
ethyl myristate	5134	6822	2158	1941	0	5011	4457	7979
2-ethyl-phenol	4988	23550	3610	5952	4567	5760	3978	16333
2-methoxy-4-vinylphenol	8231	7314	8512	8128	14084	6770	6436	6699
ethyl palmitate	2416	2747	1896	1462	2118	3506	2004	2934
(e)-ethyl 9-octadecenoate	59965	52907	67826	68332	76066	52358	64639	50033
ethyl linoleate	16425	17059	14357	15194	17187	19994	17840	16716

Table S3. Continued.

Volatile	Timepoint							
	2	2	2	2	5	5	5	5
ethyl acetate	1232698	1620605	1370007	1873927	1675672	1553291	1508095	1164956
acetal	8006	15941	12486	14191	21618	21141	15789	17239
2-butanone	170596	211682	181422	258214	281938	256310	228218	170528
2-methyl-butanal	100213	156881	151394	185407	15501	9181	19199	6288
3-methyl-butanal	171417	251045	232506	321600	70210	54988	84453	52793
2-ethyl-furan	277638	273362	260357	238926	242348	187535	227479	174711
2,4,5-trimethyl-1,3-dioxolane	2294	3645	3184	3793	3700	4319	4011	3531
pentanal	329517	474746	534818	510964	110819	94083	138564	117686
ethyl butyrate	20867	18349	17205	21922	23777	20990	19986	15928
ethyl 2-methylbutyrate	3565	3431	3014	4206	4795	5500	3589	3432
ethyl isovalerate	1678	1814	1084	1280	1475	1551	1425	1915
hexanal	277277	377601	515190	582846	85956	95935	125045	110891
2-methyl-1-propanol	25324	30505	20427	19439	49783	61872	37736	37218
isoamyl acetate	4606	13031	8116	9105	11006	13079	8432	11991
2-heptanone	71327	85925	85809	41080	52601	27366	42524	82977
3-methyl-1-butanol	154686	111467	79872	73100	189427	185430	109299	142172
2-pentyl-furan	217692	867333	964022	484742	709588	351155	504633	827349
ethyl hexanoate	627	0	0	0	0	0	0	0
3-methyl-3-buten-1-ol	12650	12290	11078	10153	21753	20561	16780	17746
1-pentanol	372126	392736	369061	288413	566263	516730	387639	472416
3-octanone	2566	6963	5316	4301	6164	8261	4839	7604
acetoin	372464	948762	386648	164757	1560958	1405962	508021	799129
ethyl lactate	20051	37877	16801	19200	31213	40748	20392	38052
3-pentanol	6210	23318	8402	8627	13029	16109	11598	16404
1-hexanol	1038246	984814	859290	692146	1337918	1379457	1080397	1402269
2-hydroxy-3-pentanone	11602	19376	9753	10542	17248	21800	12542	21177
4-hydroxy-4-methyl-2-pentanone	54608	133343	251605	64310	86892	74157	132593	98816
diethyl-acetic acid	1116	2189	834	1359	2422	3860	1654	1907
3-ethoxy-1-propanol	5108	6461	2930	4415	7494	9990	5355	6796
acetoin acetate	7944	10141	7181	5248	8746	10358	6642	9713
2-nonanone	4037	7421	3832	5775	6828	9192	6784	12117
2-methyl-1-butanol	21100	15500	9836	9674	9509	21274	9754	14645
1,3-di-tert-butylbenzene	45658	43556	43232	32305	44150	47922	39196	47013
2,2-dimethyl-3-heptanone	2268	6214	3232	3609	5722	9527	3924	6211
acetic acid	200220	197563	189239	136240	185956	203954	174685	229426
tetramethyl-pyrazine	1946	5408	0	4229	6516	12090	6163	6646
3-oxobutan-2-yl 2-methylbutanoate	338	1360	0	337	647	1644	197	915
propanoic acid	6135	16082	3119	2406	8660	13317	9648	14366
ethyl 2-hydroxy-4-methylvalerate	3614	3826	2605	3331	5400	6249	5410	5273
2-methyl-propanoic acid	21635	653175	52951	6752	22589	26770	26457	283096
caryophyllene	1746	1167	1060	408	1079	1571	1457	2078
2-furanmethanol	13120	14160	13040	8746	13091	11731	14807	15256
2-methyl-butanoic acid	33393	463325	62396	17013	58388	75053	72004	293685
3-methyl-butanoic acid	42267	249905	43188	10960	19795	36778	20508	196293
ethyl phenylacetate	5790	2734	565	2905	2075	5678	2131	2532
hexanoic acid	42210	51509	56965	31043	83563	106768	129901	139993
mequinol	5951	21760	6014	4144	6509	6600	7209	16577
benzyl alcohol	6954	8284	5765	2751	2591	2765	6857	11847
phenylethyl alcohol	114793	59406	15134	37017	43029	92596	28544	59066
ethyl myristate	4586	5207	1353	6740	5833	9696	6006	6722
2-ethyl-phenol	16188	13184	15921	12100	234025	283543	293122	344066
2-methoxy-4-vinylphenol	8080	35662	8646	5290	9714	9341	10531	17963
ethyl palmitate	4927	4454	1679	3565	2672	4045	2711	4189
(e)-ethyl 9-octadecenoate	65354	62538	71433	43424	57111	44564	53243	66593
ethyl linoleate	25196	17348	15555	20015	16593	16604	14872	19650

Table S3. Continued.

Volatile	Timepoint							
	5	5	12	12	12	12	12	12
ethyl acetate	1224756	1326925	1356379	931612	668758	760946	870367	754370
acetal	12935	13415	22812	14462	11796	5598	8930	13508
2-butanone	178575	187234	267015	213489	135815	147246	160644	140343
2-methyl-butanal	5090	18348	442	338	47	479	0	229
3-methyl-butanal	49243	75042	12686	7934	6363	10859	11098	11169
2-ethyl-furan	169320	208402	159063	76972	82320	151302	130676	162303
2,4,5-trimethyl-1,3-dioxolane	3487	2930	3240	3588	1940	3749	2620	2410
pentanal	113734	157335	36708	29909	20146	31632	31286	35173
ethyl butyrate	16289	14804	21853	28912	12626	22277	19624	14785
ethyl 2-methylbutyrate	3067	3113	4627	4313	2792	5252	4416	2793
ethyl isovalerate	1101	638	2495	3376	1208	1353	1018	1358
hexanal	67807	105254	28915	20101	15048	21717	22139	35928
2-methyl-1-propanol	21923	30003	61322	55706	41390	27051	20529	37492
isoamyl acetate	8537	7133	9234	10307	7039	6967	5731	8525
2-heptanone	120794	94311	76478	87487	36133	148389	173079	130499
3-methyl-1-butanol	157857	138992	184872	216202	115675	186638	159714	146796
2-pentyl-furan	713399	850251	620893	560445	217415	1117722	1097979	817123
ethyl hexanoate	1238	1030	0	0	0	4920	4416	0
3-methyl-3-buten-1-ol	21495	19495	29113	31463	22154	27891	27613	26520
1-pentanol	606307	539300	604070	654922	384429	557412	572133	546467
3-octanone	6065	6523	7240	10339	5507	8635	7986	8843
acetoin	827255	494407	555437	651035	311163	520288	470174	403705
ethyl lactate	22254	19469	27460	32344	23629	28473	19805	20054
3-pentanol	13185	13409	14978	17791	12788	10630	12331	13797
1-hexanol	1907124	1601523	1418495	1650532	1062405	1423830	1552154	1570834
2-hydroxy-3-pentanone	15341	13338	16364	18569	14395	14508	13080	13388
4-hydroxy-4-methyl-2-pentanone	89977	80961	94830	1401771	73466	289755	58227	110727
diethyl-acetic acid	1536	1387	2907	3441	2185	1703	1479	1573
3-ethoxy-1-propanol	3588	3206	6954	12462	5986	6122	3290	3785
acetoin acetate	8766	7151	9208	17716	6381	9290	6727	6856
2-nonanone	14253	8874	23351	32879	20492	28252	33710	27458
2-methyl-1-butanol	26013	6891	10362	17845	11058	19077	16549	5379
1,3-di-tert-butylbenzene	62686	50591	46442	53461	35922	49214	51114	47740
2,2-dimethyl-3-heptanone	2156	3785	5741	7419	4266	3774	2285	3167
acetic acid	325610	271457	178731	205422	160154	204939	234824	235222
tetramethyl-pyrazine	1798	2076	7260	10400	7855	3780	1749	2891
3-oxobutan-2-yl 2-methylbutanoate	667	363	966	1331	439	556	453	566
propanoic acid	14910	7280	17617	24876	13083	26774	16215	16456
ethyl 2-hydroxy-4-methylvalerate	6063	4941	6223	6751	4717	6594	5797	6005
2-methyl-propanoic acid	227967	75794	34982	44707	21884	61526	63389	62084
caryophyllene	3627	1928	601	1146	464	1506	1736	1868
2-furanmethanol	19807	13925	14467	17664	10790	18471	17378	18501
2-methyl-butanoic acid	239373	106977	84342	112946	60686	100499	100587	110501
3-methyl-butanoic acid	151646	60582	22235	19694	13448	65905	50593	47180
ethyl phenylacetate	1985	869	803	3376	2006	5495	1268	917
hexanoic acid	154402	89361	143018	215167	137312	140703	117869	150835
mequinol	14004	8030	6335	7083	4550	6993	7754	8011
benzyl alcohol	14815	9347	3449	5764	6569	15350	13825	15617
phenylethyl alcohol	50549	21176	14114	57402	28031	114521	37391	23910
ethyl myristate	2743	2682	5199	8656	12090	6562	2620	1979
2-ethyl-phenol	554552	356263	403115	510079	302063	450109	489814	495964
2-methoxy-4-vinylphenol	19705	11808	9830	11517	6141	10717	10842	10517
ethyl palmitate	3436	1942	3017	3667	3873	5550	2880	2056
(e)-ethyl 9-octadecenoate	70364	71470	57425	51506	44148	79610	70488	61896
ethyl linoleate	16164	15976	15479	15790	20965	20027	16985	16087

Table S3. Continued.

Volatile	Timepoint							
	24	24	24	24	24	24	48	48
ethyl acetate	496055	303896	268827	352192	167103	524100	171988	133999
acetal	18903	11904	9882	10973	10273	10360	16768	7694
2-butanone	163815	107691	81415	113113	63604	141804	105114	75889
2-methyl-butanal	1042	2357	595	122	707	523	1025	442
3-methyl-butanal	6490	11304	3511	3378	3344	9003	4123	2080
2-ethyl-furan	39597	31943	32488	57520	24059	111904	25331	21542
2,4,5-trimethyl-1,3-dioxolane	3006	3812	1620	1699	1862	3187	4364	2634
pentanal	34538	29909	21611	22535	21261	38969	41318	28651
ethyl butyrate	23371	21285	12700	13364	14013	17482	16813	11784
ethyl 2-methylbutyrate	4821	3742	3370	3120	3548	3567	4049	2810
ethyl isovalerate	1098	1682	2165	1837	2706	1483	1278	1869
hexanal	10382	9441	13481	9366	13637	23452	8711	11094
2-methyl-1-propanol	51687	51524	35688	28408	30809	18078	31020	27868
isoamyl acetate	5863	10747	7456	8120	8718	6254	6422	6826
2-heptanone	194089	200666	144766	68156	107247	358077	288922	226107
3-methyl-1-butanol	196135	248947	130928	104421	144199	167594	167859	112838
2-pentyl-furan	560798	502051	444624	266552	338934	1131377	311654	275968
ethyl hexanoate	2741	2399	0	0	0	4444	753	0
3-methyl-3-buten-1-ol	65173	54405	41774	32235	37762	52508	127232	97249
1-pentanol	639796	529307	386610	336970	328023	632299	428726	321860
3-octanone	7597	7606	6985	7599	7050	15213	10964	7460
acetoin	827197	881654	584936	330978	452200	586957	556211	443671
ethyl lactate	26234	39265	20442	22349	37670	18774	33130	20536
3-pentanol	11876	12028	9366	10188	9241	11372	10976	8613
1-hexanol	1273583	1192758	942598	881267	837085	1685338	1112329	864095
2-hydroxy-3-pentanone	14970	21181	11891	12934	16158	13328	16302	11373
4-hydroxy-4-methyl-2-pentanone	91283	2565265	117162	81099	95595	176669	34380	45327
diethyl-acetic acid	2499	3117	1596	2775	2456	2045	4398	3105
3-ethoxy-1-propanol	5479	16518	5025	5404	7308	3794	7101	4797
acetoin acetate	9083	23311	6778	6453	6722	9307	12472	9192
2-nonanone	56884	65751	46473	35989	45804	75671	104006	80240
2-methyl-1-butanol	8268	20870	7628	10321	14812	19016	13817	9692
1,3-di-tert-butylbenzene	43636	42989	33641	37343	32999	63145	40075	32595
2,2-dimethyl-3-heptanone	4938	8742	3370	4321	5781	2314	5231	3312
acetic acid	154094	159714	132658	131474	117137	244157	153894	129404
tetramethyl-pyrazine	5686	12416	6541	7928	9597	2446	7881	6886
3-oxobutan-2-yl 2-methylbutanoate	795	1140	594	773	603	587	926	624
propanoic acid	22886	41067	18482	13580	22692	27587	30865	24410
ethyl 2-hydroxy-4-methylvalerate	6060	7177	5384	5496	6316	6705	8120	5612
2-methyl-propanoic acid	41805	69424	33207	21061	44633	73595	50047	38162
caryophyllene	426	1339	389	292	662	1816	767	480
2-furanmethanol	13748	17681	12740	10470	13765	21122	15191	13204
2-methyl-butanoic acid	68620	107314	59918	42560	74407	112910	55079	44331
3-methyl-butanoic acid	25413	41069	25857	14981	64472	48881	26073	20900
ethyl phenylacetate	1081	7617	1628	2516	2693	485	5718	1341
hexanoic acid	121832	148218	90543	83674	123214	184708	109454	103552
mequinol	4056	4691	4051	3368	3319	6975	3232	2622
benzyl alcohol	3401	10428	8743	6880	10100	20030	10728	10675
phenylethyl alcohol	18540	138744	38275	33622	94229	27855	88319	30908
ethyl myristate	4795	8695	7283	6198	8256	2761	8077	7275
2-ethyl-phenol	285013	332409	265180	228476	229007	467805	210335	165048
2-methoxy-4-vinylphenol	6976	8488	7052	4045	4936	9330	3138	3256
ethyl palmitate	2840	5802	3957	4057	5391	2188	3804	3647
(e)-ethyl 9-octadecenoate	61481	59801	43932	39906	45185	69237	53057	46357
ethyl linoleate	17324	19643	20359	20254	21196	17860	15332	21791

Table S3. Continued.

Volatile	Timepoint							
	48	48	48	48	72	72	72	72
ethyl acetate	111319	124420	147830	137341	127792	104420	85211	112287
acetal	11406	10638	11699	11510	17226	19324	13141	9197
2-butanone	68428	71197	77177	76212	72508	54666	37535	55000
2-methyl-butanal	541	437	575	1076	2048	1941	1216	1274
3-methyl-butanal	3159	3363	7122	5291	4532	4401	6045	4663
2-ethyl-furan	23110	17711	30404	37560	21531	7996	10766	25324
2,4,5-trimethyl-1,3-dioxolane	2726	2254	2960	3900	2591	2960	2157	2090
pentanal	28407	27909	52367	46071	40468	35482	36166	36406
ethyl butyrate	10132	13490	18543	20218	21968	18834	19470	19817
ethyl 2-methylbutyrate	3531	3232	4548	5323	4619	5155	5866	5787
ethyl isovalerate	2009	1784	1252	1436	1668	2219	1594	844
hexanal	9556	7514	19626	13167	13601	20730	20099	22930
2-methyl-1-propanol	21887	22390	31853	32404	37864	25992	27386	25627
isoamyl acetate	5170	4984	7375	7431	11563	10136	6416	5356
2-heptanone	144908	247076	772263	654072	220643	170592	356421	282292
3-methyl-1-butanol	93916	103730	188348	184519	205148	189717	202283	130773
2-pentyl-furan	187898	342570	814517	871444	282829	218881	555658	580826
ethyl hexanoate	0	2989	5401	4040	2275	3440	2748	10384
3-methyl-3-buten-1-ol	79218	93760	151122	138920	171755	171501	156740	153880
1-pentanol	271583	306977	551936	516174	420106	454839	424453	389579
3-octanone	8241	9026	15110	15483	10756	13117	7805	16174
acetoin	320515	369450	642719	572050	731806	646429	814757	541737
ethyl lactate	22326	20226	23763	30228	57980	61965	27389	24818
3-pentanol	8195	8101	11231	12263	11170	13971	10938	10295
1-hexanol	775839	777030	1416282	1424802	1139821	1176722	1070346	1046959
2-hydroxy-3-pentanone	12421	11459	14090	15376	29669	28205	14764	13046
4-hydroxy-4-methyl-2-pentanone	53498	24995	92023	206570	82806	80062	125889	83205
diethyl-acetic acid	3172	2836	3511	3952	5369	4562	2812	3093
3-ethoxy-1-propanol	5319	4479	5555	7022	12733	13317	7131	4901
acetoin acetate	8605	8858	15779	16522	15518	14862	11642	10393
2-nonanone	74879	68479	182668	170660	142866	127682	123004	99683
2-methyl-1-butanol	13238	13669	10716	16941	36004	40224	10280	9913
1,3-di-tert-butylbenzene	31258	30904	56655	56488	43709	48806	40986	42238
2,2-dimethyl-3-heptanone	4590	4501	5209	6666	13541	14030	4996	5165
acetic acid	116654	115898	220606	246440	186271	200557	181043	185155
tetramethyl-pyrazine	8897	6279	5391	7910	18265	17599	5265	3379
3-oxobutan-2-yl 2-methylbutanoate	818	537	887	1211	1939	2330	827	793
propanoic acid	19399	19591	46298	29294	37264	32329	41443	33737
ethyl 2-hydroxy-4-methylvalerate	5557	5762	8683	9123	9568	12737	7356	7991
2-methyl-propanoic acid	27686	30452	70931	58050	69261	42270	66621	58759
caryophyllene	471	494	1452	2151	1680	2245	1636	1398
2-furanmethanol	12432	12874	24596	20636	18559	18484	22671	19412
2-methyl-butanoic acid	41348	37337	75979	70796	72023	49945	66427	60707
3-methyl-butanoic acid	11003	17619	36680	57181	80639	36726	33180	41133
ethyl phenylacetate	775	797	2541	2854	6788	11090	4174	3567
hexanoic acid	91510	75186	177620	132203	119761	110511	135727	126603
mequinol	2658	2550	4241	4329	2877	2901	3528	3093
benzyl alcohol	10595	9230	22497	20288	12902	12723	20221	18785
phenylethyl alcohol	17966	17468	81020	80759	172165	205077	153352	74182
ethyl myristate	8406	6786	6253	6907	10624	10453	6400	4578
2-ethyl-phenol	161727	149003	289249	290270	176120	195124	243327	192543
2-methoxy-4-vinylphenol	2573	2460	4903	4369	3629	4566	6124	3303
ethyl palmitate	4341	4013	3856	3531	5832	5743	4229	3761
(e)-ethyl 9-octadecenoate	41568	46640	77586	64323	57621	51734	73877	76691
ethyl linoleate	21646	21031	19011	17398	19279	17668	20512	18716

Table S3. Continued.

Volatile	Timepoint							
	72	72	120	120	120	120	120	120
ethyl acetate	123879	103042	102554	94077	110539	75646	76195	87170
acetal	11778	11555	11180	17247	11908	9215	8765	18258
2-butanone	59267	51538	45261	41832	43188	28110	25877	32044
2-methyl-butanal	859	872	968	1288	1715	445	946	1340
3-methyl-butanal	6256	6682	5089	7501	9356	5761	5984	8068
2-ethyl-furan	29317	21535	13114	8937	9208	8249	8901	8418
2,4,5-trimethyl-1,3-dioxolane	2257	2552	2471	2938	2524	1965	3068	1876
pentanal	37600	43744	31585	32202	33934	30381	29312	32087
ethyl butyrate	16711	15850	18487	17055	17253	16113	15394	14482
ethyl 2-methylbutyrate	3767	4112	3677	4373	4848	3899	3393	4125
ethyl isovalerate	1054	1037	1074	965	1003	513	387	801
hexanal	32206	31719	19280	67409	45110	31665	35297	34649
2-methyl-1-propanol	22669	26476	20134	30980	30187	12319	19621	16069
isoamyl acetate	6092	5739	8611	6546	5648	3598	4059	4284
2-heptanone	341834	530137	209621	123544	219342	183786	205211	196926
3-methyl-1-butanol	122883	143023	126747	117446	152078	105434	102686	99564
2-pentyl-furan	713610	506407	436122	219858	423042	318642	357160	322134
ethyl hexanoate	1869	11540	2330	948	1548	1364	1858	932
3-methyl-3-buten-1-ol	173393	172608	182726	170645	167995	130501	127073	134964
1-pentanol	435184	482451	395146	372292	424042	333131	314980	338332
3-octanone	14414	12943	14206	15712	8291	6292	7812	7311
acetoin	507620	808844	1127495	1282778	1144840	947092	849667	1074323
ethyl lactate	19551	20030	26593	65322	28101	19688	20194	22782
3-pentanol	10733	12541	14286	14852	11240	7582	8410	10114
1-hexanol	1285568	1211760	1011231	989860	1008965	726893	745928	823472
2-hydroxy-3-pentanone	12599	14258	16696	36522	14931	10440	11374	12898
4-hydroxy-4-methyl-2-pentanone	200518	150831	151734	39824	87968	92824	187592	65692
diethyl-acetic acid	3418	2768	15071	12842	4485	4129	3975	4799
3-ethoxy-1-propanol	4127	5283	5130	10307	5309	2824	3777	3703
acetoin acetate	11139	14099	14051	15143	11482	9090	10399	10576
2-nonanone	120802	142452	114319	108381	125985	88667	105980	106567
2-methyl-1-butanol	7494	12900	11340	40970	11176	5906	8449	8606
1,3-di-tert-butylbenzene	51035	45361	37852	37013	40778	30001	31072	31309
2,2-dimethyl-3-heptanone	4088	5693	5101	15135	4627	2539	2963	3173
acetic acid	245679	197160	184588	193716	195735	131902	147778	159707
tetramethyl-pyrazine	4829	8432	5961	17583	6194	2784	3593	3554
3-oxobutan-2-yl 2-methylbutanoate	714	980	868	2098	1086	492	0	623
propanoic acid	27854	43632	37896	37777	39662	37969	34489	29275
ethyl 2-hydroxy-4-methylvalerate	7904	6701	8411	8813	8270	6319	5513	6740
2-methyl-propanoic acid	66296	85836	82781	167945	95359	72406	83629	65370
caryophyllene	1605	1284	1057	1279	1605	525	1183	818
2-furanmethanol	19310	22153	20958	19975	22512	19355	17657	18983
2-methyl-butanoic acid	63307	78190	80367	171727	92370	55654	70156	51234
3-methyl-butanoic acid	30226	32787	59503	137806	73538	39944	40197	33118
ethyl phenylacetate	1056	754	1586	1248	2203	615	1010	743
hexanoic acid	123129	162892	113042	132045	145505	121636	123935	115803
mequinol	3463	3522	3342	8275	4279	3023	2457	2433
benzyl alcohol	20574	20884	17812	17193	19738	14948	17380	16982
phenylethyl alcohol	33171	28022	43887	26093	73981	27814	34636	23163
ethyl myristate	3024	4735	5519	5977	4894	3777	3185	3740
2-ethyl-phenol	219018	235053	160441	175275	221404	144603	168027	168043
2-methoxy-4-vinylphenol	3399	4575	3343	14199	6312	3623	3018	2888
ethyl palmitate	2156	2631	3244	3313	3761	2762	2636	2276
(e)-ethyl 9-octadecenoate	72986	76165	69557	69857	67267	81399	71824	73567
ethyl linoleate	16913	15758	18520	22678	19281	18469	16878	15272