

**Supplementary Materials for
Metabolomic Profiling of Sweat VOCs for Occupational Stress Surveillance in
Firefighters: A GC-MS Pilot Study**

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Contents

Supplementary Table 1 Perceived stress scores (PSS) of controls and high stress volunteers

Supplementary Table 2 Volatile compound profile data (average areas of different peaks) of control and high stress samples analyzed using HS-SPME GC-MS. Unknown identities were identified with retention time in min.

Supplementary Table 1 Perceived stress scores (PSS) of controls and high stress volunteers

Control volunteer code	PSS	High stress volunteer code	PSS
F0132	16	F0215	32
F0144	15	F0216	32
F0148	16	F0220	32
F0152	16	F0235	32
F0153	18	F0244	33
F0155	18	F0252	33
F0157	18	F0267	33
F0158	18	F0270	33
F0159	19	F0273	33
F0165	19	F0277	34
F0168	20	F0282	34
F0176	20	F0284	34
F0177	20	F0292	35
F0178	20	F0295	35
F0183	20	F0297	35
F0186	23	F0338	36
F0193	23	F0356	36
F0195	26	F0364	36
F0199	26	F0369	36
F0204	27	F0378	36
F0212	30	F0382	39
		F0420	39

Supplementary Table 2 Volatile compound profile data (average areas of different peaks) of control and high stress samples analyzed using HS-SPME GC-MS. Unknown identities were identified with retention time in min.

No.	Compound or retention time (min) for unknown	Literature RI	Experimental RI	Average peak area (counts)		Biological evidence / example microbiome(s) producing the compound
				Control Samples	High stress Samples	
1	4.7	-	802	154	0	-
2	Butanoic acid	805	803	0	0	Butanoic acid found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Torulaspora Delbrueckii</i> , <i>Peribacillus Sp.</i> , <i>Psychrobacillus Vulpis</i>
3	5	-	818	1643	0	-
4	5.4	-	830	130935	91090	-
5	5.8	-	848	0	548	-
6	6.1	-	861	14766	0	-
7	6.2	-	862	3745	0	-
8	7.2	-	903	639	0	-
9	1-Nonene / ^a Pentanoic acid	889 / 901	904	436	446	1-Nonene found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Pseudomonas Aeruginosa</i> , <i>Pseudomonas Fluorescens</i> , <i>Pseudomonas Azotoformans</i> , <i>Trichoderma Atroviride</i> Pentanoic acid found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Bacillus Amyloliquefaciens</i> , <i>Bacillus Toyonensis</i> , <i>Bacillus Mycoides</i> , <i>Serratia Fonticola</i>
10	7.3	-	907	390	0	-
11	8	-	926	23161	0	-
12	8.1	-	929	0	20275	-
13	8.2	-	932	52537	7069	-
14	8.2	-	933	23724	0	-

15	8.5	-	943	869	0	-
16	8.9	-	954	56292	2998	-
17	9.1	-	960	920	3018	-
18	9.3	-	966	600	0	-
19	9.9	-	986	0	5729	-
20	9.9	-	987	11743	862	-
21	10	-	988	0	1308	-
22	Octanal	1003	991	36504	21556	Octanal found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Zygosaccharomyces Rouxii</i>
23	10.1	-	992	0	1613	-
24	11	-	1017	4874	3854	-
25	11.1	-	1019	4067	0	-
26	11.2	-	1024	1459	504	-
27	11.2	-	1025	247	0	-
28	11.3	-	1026	2319	0	-
29	11.4	-	1028	1227	0	-
30	11.4	-	1029	989	965	-
31	<i>p</i> -Cymene / Eucalyptol	1025 / 1032	1032	1805	4345	<i>p</i> -Cymene found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Mycobacterium Tuberculosis</i> , <i>Fusarium Culmorum</i> , <i>Amanita Ovoidea</i> , <i>Mycena Rosea</i> Eucalyptol found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Hypoxylon Anthochroum</i> , <i>Erwinia Amylovora</i> , <i>Hypoxylon Anthochroum</i> , <i>Gloeophyllum Odoratum</i>
32	d-Limonene	1031	1033	4098	3106	d-Limonene found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Aspergillus Fumigatus</i> , <i>Escherichia Coli</i> ,

						<i>Burkholderia Tropica</i> , <i>Staphylococcus Equorum</i>
33	11.6	-	1034	0	0	-
34	11.6	-	1036	3448	1732	-
35	11.9	-	1045	0	266	-
36	12.3	-	1054	1516	0	-
37	12.3	-	1055	610	0	-
38	Decane, 2,6,7-trimethyl-	1058	1056	1916	0	Decane, 2,6,7-trimethyl- found in: 1. mVOC database / <i>Paenibacillus Polymyxa</i>
39	Decane, 2-methyl-	1064	1059	4537	1360	Decane, 2-methyl- found in: 1. mVOC database / <i>Streptomyces Philanthi</i>
40	12.5	-	1060	670	0	-
41	12.6	-	1064	697	0	-
42	12.7	-	1066	1185	974	-
43	7-Octen-2-ol, 2,6-dimethyl-	1064	1074	4996	19544	7-Octen-2-ol, 2,6-dimethyl- found in: 1. mVOC database / <i>Candida Albicans</i> , <i>Candida Glabrata</i> , <i>Candida Tropicalis</i> , <i>Saccharomyces Cerevisiae</i>
44	Decane, 4-methyl-	1060	1078	891	1226	Decane, 4-methyl- found in: 1. mVOC database / <i>Saccharomyces Cerevisiae</i>
45	13.4	-	1087	44457	29774	-
46	13.5	-	1088	97580	82383	-
47	Pyrazine, tetramethyl-	1089	1091	0	0	Pyrazine, tetramethyl- found in: 1. mVOC database / <i>Pseudomonas Aeruginosa</i> , <i>Bacillus Subtilis</i> , <i>Coralitalea Coralii</i> , <i>Bacillus Sp.</i>
48	13.7	-	1093	2072	0	-
49	1-Undecene	1091	1095	5484	0	1-Undecene found in: 1. mVOC database / <i>Staphylococcus Aureus</i> , <i>Staphylococcus Epidermidis</i>
50	Hydroxylamine, O-decyl-	1100	1098	2710	3301	Hydroxylamine, O-decyl- found in: 1. mVOC database / <i>Stenotrophomonas Maltophilia</i>

51	14	-	1101	2739	4536	-
52	10.5 / 3-Octanol, 3,7-dimethyl-	1100	1103	22716	1873	3-Octanol, 3,7-dimethyl- found in: 1. mVOC database / <i>Candida Albicans</i> , <i>Candida Glabrata</i> , <i>Candida Tropicalis</i>
53	3-Carene	1101	1104	3821	8143	3-Carene found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Candida Albicans</i> , <i>Candida Glabrata</i> , <i>Candida Tropicalis</i> , <i>Fusarium Graminearum</i>
54	14.1	-	1105	9699	0	-
55	14.2	-	1110	753	0	-
56	2-Nonen-1-ol	1105	1115	0	3900	2-Nonen-1-ol found in: 1. mVOC database / <i>Serratia Proteamaculans</i> , <i>Rhizoctonia Solani</i> , <i>Lactobacillus Plantarum</i> , <i>Bacillus Safensis</i>
57	2-Nonanol	1101	1116	386	698	2-Nonanol found in: 1. mVOC database / <i>Pseudomonas Aeruginosa</i> , <i>Pseudomonas Sp.</i> , <i>Pseudomonas Azotoformans</i> , <i>Escherichia Coli</i>
58	Nonanal	1104	1119	14590	16000	Nonanal found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Streptococcus Pneumoniae</i>
59	2-Nonanol / 14.6	1101	1120	17091	10048	2-Nonanol found in: 1. mVOC database / <i>Pseudomonas Aeruginosa</i> , <i>Pseudomonas Sp.</i> , <i>Pseudomonas Azotoformans</i> , <i>Escherichia Coli</i>
60	14.7	-	1121	0	738	-
61	14.8	-	1124	0	1853	-
62	14.8	-	1125	1689	0	-
63	14.8	-	1126	10868	15468	-
64	14.9	-	1127	9279	6479	-
65	15	-	1132	8646	71541	-
66	15.2	-	1136	1476	3477	-

67	15.3	-	1138	1605	3309	-
68	15.3	-	1139	0	1000	-
69	15.4-15.5	-	1143	54324	231794	-
70	trans-Verbenol	1144	1145	0	2518	trans-Verbenol found in: 1. mVOC database / <i>Entomocorticium Sp.</i>
71	Camphor	1145	1146	40048	47912	Camphor found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Tuber Melanosporum, Ganoderma Lucidum, Meyerozyma Guilliermondii, Saccharomyces Cerevisiae</i>
72	15.6	-	1147	6783	17556	-
73	15.8	-	1154	574	0	-
74	15.9	-	1157	0	791	-
75	16.2	-	1164	1568	964	-
76	16.3	-	1166	0	1946	-
77	Isoborneol / (+)-Borneol	1157 / 1168	1167	12217	6268	Isoborneol found in: 1. KEGG COMPOUND Database (+)-Borneol found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Candida Albicans, Candida Glabrata, Candida Tropicalis, Nannocystis Exedens</i>
78	16.3	-	1168	1083	659	-
79	Undecane, 3-methyl-	1170	1172	3678	2454	Undecane, 3-methyl- found in: 1. mVOC database / <i>Fusarium Graminearum, Microbacterium</i>
80	15.5	-	1173	8635	2066	-
81	dl-Menthol / Levomenthol	1173 / 1175	1175	72148	69208	dl-Menthol found in: 1. mVOC database / <i>Cytophaga-Flavobacterium-Bacteroides, Stigmatella Aurantiaca, Serratia Proteamaculans, Carnobacterium Divergens</i>

						Levomenthol found in: 1. mVOC database / <i>Cytophaga-Flavobacterium- Bacteroides, Stigmatella Aurantiaca, Serratia Proteamaculans, Carnobacterium Divergens</i>
82	16.6	-	1177	0	11768	-
83	16.9	-	1183	3342	0	-
84	16.9	-	1184	0	17337	-
85	16.6	-	1187	8445	0	-
86	17	-	1188	727	0	-
87	17.2	-	1193	18938	137637	-
88	17.3	-	1194	89699	13889	-
89	17.3	-	1196	8782	4666	-
90	17.4	-	1197	2374	41274	-
91	17.5	-	1201	27665	23348	-
92	17.5	-	1202	29942	14846	-
93	17.6	-	1203	994	802	-
94	Decanal / 17.8	1206	1211	17352	54124	Decanal found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Pseudomonas Putida</i>
95	17.9	-	1213	3452	3751	-
96	18	-	1216	9085	16697	-
97	18.1	-	1218	0	4017	-
98	18.3	-	1225	1018	0	-
99	2-Ethylhexyl acrylate	1220	1232	96897	147326	2-Ethylhexyl acrylate found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Saccharomyces Cerevisiae</i>
10 0	18.7	-	1237	1008	15377	-
10 1	18.8	-	1238	5752	0	-
10 2	Neral	1240	1239	0	917	Neral found in: 1. KEGG COMPOUND Database 2. mVOC database /

						<i>Aspergillus Fumigatus,</i> <i>Ganoderma Lucidum,</i> <i>Gloeophyllum Odoratum,</i> <i>Saccharomyces Cerevisiae</i>
10 3	18.9	-	1243	350	3038	-
10 4	19	-	1244	9966	0	-
10 5	19	-	1246	0	781	-
10 6	19.1	-	1248	3271	0	-
10 7	19.2	-	1250	99207	0	-
10 8	19.5	-	1259	1274217	0	-
10 9	19.6	-	1263	1581758	0	-
11 0	19.7	-	1264	1631655	4574608	-
11 1	20.1	-	1278	0	5032798	-
11 2	20.2	-	1279	0	4475679	-
11 3	Dodecane, 2,6,11- trimethyl-	1275	1281	1494	0	Dodecane, 2,6,11-trimethyl- found in: 1. mVOC database / <i>Klebsiella</i> <i>Pneumoniae</i> , <i>Bacillus</i> <i>Amyloliquefaciens</i> , <i>Pseudomonas</i> <i>Brassicacearum</i> , <i>Pseudomonas Putida</i>
11 4	20.3	-	1283	0	23734594	-
11 5	20.4	-	1286	19066112	12413196	-
11 6	20.5 ^b	-	1288	0	47248671	-
11 7	20.6	-	1291	30975448	26896489	-
11 8	20.7	-	1293	41987406	5874634	-
11 9	20.7	-	1294	26963627	0	-
12 0	20.8	-	1296	13378941	25026655	-

12 1	20.9	-	1300	20268955	61267	-
12 2	21.1	-	1307	1502	0	-
12 3	Undecanal	1307	1309	0	0	Undecanal found in: 1. mVOC database / <i>Escherichia Coli</i> , <i>Pseudomonas Aeruginosa</i> , <i>Erwinia Amylovora</i> , <i>Streptococcus Mutans</i>
12 4	21.2	-	1311	0	1365	-
12 5	21.4	-	1316	12908	2150	-
12 6	21.6	-	1321	2619	0	-
12 7	21.7	-	1325	15869	0	-
12 8	21.8	1341	1327	36850	19260	-
12 9	22.1	-	1337	0	1263	-
13 0	22.3	-	1344	9498	6439	-
13 1	22.4	-	1347	2826	819	-
13 2	Triacetin	1350	1370	90074951	16673298 6	Triacetin found in: 1. mVOC database / <i>Bacillus Toyonensis</i> , <i>Pleurotus Ostreatus</i> , <i>Microbacterium</i>
13 3	23.2	-	1371	4588	17645	-
13 4	23.2	-	1372	16768584 5	14269843 8	-
13 5	23.3	-	1375	51026905 6	19397086 6	-
13 6	23.4	-	1377	21998707 2	21970814 9	-
13 7	23.5	-	1378	55499234	16076320 8	-
13 8	23.7	-	1387	0	25729391	-
13 9	23.9	-	1392	98724273	24803425 4	-

14 0	Butyl caprylate	1389	1394	14331	0	Butyl caprylate found in: 1. mVOC database / <i>Saccharomyces Cerevisiae</i>
14 1	Decane, 2,3,5-trimethyl-	1411	1400	34499	0	Decane, 2,3,5-trimethyl- found in: 1. mVOC database / <i>Meyerozyma Guilliermondii</i>
14 2	24.2	-	1402	381802	547073	-
14 3	24.3	-	1404	28846	19285	-
14 4	24.4	-	1408	2287	0	-
14 5	24.5	-	1409	79049	1929	-
14 6	Phenol, 4-(1,1-dimethylpropyl)-	1400	1411	0	0	Phenol, 4-(1,1-dimethylpropyl)- found in: 1. mVOC database / <i>Mycobacterium Tuberculosis</i>
14 7	24.6	-	1415	19840	0	-
14 8	Dodecanal	1409	1417	51498	130636	Dodecanal found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Aspergillus Niger, Candida Albicans, Penicillium Chrysogenum</i>
14 9	24.7	-	1419	0	4712	-
15 0	24.9	-	1423	21964	32652	-
15 1	Caryophyllene	1419	1424	9837	0	Caryophyllene found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Candida Albicans, Candida Glabrata, Antrodia Cinnamomea</i>
15 2	24.9	-	1425	0	1701	-
15 3	25.1	-	1431	30477	100178	-
15 4	25.1	-	1433	0	0	-
15 5	25.2	-	1436	4901	1205	-

15 6	25.6	-	1446	16632382	13603163	-
15 7	25.7	-	1450	0	579176	-
15 8	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	1452	1460	301560	128900	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)- found in: 1. mVOC database / <i>Bacillus Acidiceler</i> , <i>Bacillus Sp.</i> , <i>Candida Albicans</i>
15 9	26.2	-	1465	1733	0	-
16 0	26.3	-	1468	20850	21575	-
16 1	26.3	-	1469	15198	19378	-
16 2	26.3	-	1470	8167	3177	-
16 3	26.4	-	1471	2838	12302	-
16 4	2-Dodecenal / 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	1465 / 1472	1472	103565	83803	2-Dodecenal found in: 1. mVOC database / <i>Candida Albicans</i> , <i>Serratia Proteamaculans</i> , <i>Carnobacterium Divergens</i> 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)- found in: 1. mVOC database / <i>Escherichia Coli</i> , <i>Metschnikowia Reukaufii</i> , <i>Debaryomyces Hansenii</i>
16 5	1,4-Benzenediol, 2,5-bis(1,1-dimethylethyl)-	1457	1473	0	5817	1,4-Benzenediol, 2,5-bis(1,1-dimethylethyl)- found in: 1. mVOC database / <i>Zygosaccharomyces Rouxii</i>
16 6	26.5	-	1474	42909	13444	-
16 7	26.6	-	1477	31766	16117	-
16 8	26.6	-	1478	0	4265	-
16 9	26.6	-	1479	24485	48220	-
17 0	2,5-di-tert-Butyl-1,4-benzoquinone	1466	1480	17030	14216	2,5-di-tert-Butyl-1,4-benzoquinone found in:

						1. mVOC database / <i>Saccharomyces Cerevisiae</i>
17 1	26.7 / 1-Dodecanol	1474	1482	39637	17025	1-Dodecanol found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Candida Dubliniensis, Candida Albicans, Escherichia Coli</i>
17 2	26.8	-	1485	29259	57794	-
17 3	26.9	-	1488	2093	3148	-
17 4	26.9	-	1490	3596	9797	-
17 5	27	-	1492	6836	16008	-
17 6	27	-	1494	0	115863	-
17 7	27.1	-	1496	3934	0	-
17 8	27.2	-	1497	121694	153116	-
17 9	27.3	-	1501	111913	157578	-
18 0	27.5	-	1509	3135	3057	-
18 1	27.6	-	1510	2381	1195	-
18 2	Tridecanal	1512	1516	15408	13212	Tridecanal found in: 1. mVOC database / <i>Escherichia Coli, Erwinia Amylovora, Pseudomonas Fragi</i>
18 3	27.7	-	1517	0	1039115	-
18 4	2,4-Di-tert-butylphenol	1519	1519	692809	506648	2,4-Di-tert-butylphenol found in: 1. mVOC database / <i>Aspergillus Niger, Candida Albicans, Penicillium Chrysogenum, Escherichia Coli</i>
18 5	1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	1524	1524	855	10663	1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)- found in: 1. mVOC database /

						<i>Aspergillus Niger,</i> <i>Algihabitans Albus</i>
18 6	28	-	1525	17281	22647	-
18 7	28.2	-	1531	4348	0	-
18 8	28.2	-	1533	35969	51887	-
18 9	28.3	-	1534	5792	6194	-
19 0	28.3	-	1537	0	2323	-
19 1	28.4	-	1538	844	0	-
19 2	28.5 / Tetradecane, 2,6,10-trimethyl-	1539	1542	122458	147575	Tetradecane, 2,6,10-trimethyl- found in: 1. mVOC database / <i>Bacillus Subtilis</i> , <i>Pseudomonas Putida</i> , <i>Staphylococcus Aureus</i>
19 3	22	-	1545	0	0	-
19 4	28.6	-	1546	0	0	-
19 5	28.7	-	1548	0	2524	-
19 6	28.7	-	1549	2835	2289	-
19 7	28.8	-	1552	81222	46087	-
19 8	28.8	-	1553	0	5599	-
19 9	Dodecanoic acid / 29	1572	1560	7631	50818	Dodecanoic acid found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Aspergillus Fumigatus</i>
20 0	29.1	1556	1561	47531	20225	-
20 1	1,6,10- Dodecatrien-3-ol, 3,7,11-trimethyl-	1563	1563	19548	15005	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl- found in: 1. mVOC database / <i>Trametes Suaveolens</i> , <i>Gloeophyllum Odoratum</i> , <i>Fomitopsis Pinicola</i> , <i>Piptoporus Betulinus</i>
20 2	29.1	-	1564	0	963	-

203	29.2	-	1565	8490	0	-
204	29.3	-	1569	839	3915	-
205	29.3	-	1570	436	0	-
206	Dodecane, 5,8-diethyl-	1572	1572	67547	69928	Dodecane, 5,8-diethyl- found in: 1. mVOC database <i>/Streptomyces Thermocarboxydus</i>
207	29.5	-	1576	802	335	-
208	29.6	-	1580	618	1162	-
209	29.7	-	1582	5944	0	-
210	29.7	-	1584	3466	11564	-
211	Caryophyllene oxide	1581	1588	132235	105045	Caryophyllene oxide found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Antrodia Cinnamomea, Trichoderma Viride, Candida Tropicalis, Candida Glabrata</i>
212	29.9	-	1589	10683	585590	-
213	30	-	1593	5661	89813	-
214	Cetene	1592	1594	0	6122	Cetene found in: 1. mVOC database / <i>Bacillus Thuringiensis, Pseudomonas Fragi, Carnobacterium Divergens, Serratia Proteamaculans</i>
215	30	-	1595	0	12114	-
216	Dodecanoic acid, ethyl ester	1594	1597	131447	14420	Dodecanoic acid, ethyl ester found in: 1. mVOC database / <i>Escherichia Coli, Bacillus Wiedmannii, Azospirillum Brasilense</i>
217	30.2	-	1599	12062	39297	-

21 8	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	1588	1600	1274172	1253351	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate found in: 1. mVOC database / <i>Saccharomyces Cerevisiae</i> , <i>Saccharomyces Eubayanus</i> , <i>Peribacillus Sp.</i>
21 9	Diethyl Phthalate	1594	1601	54948	0	Diethyl Phthalate found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Bacillus Subtilis</i> , <i>Pseudomonas Fluorescens</i> , <i>Fusarium Graminearum</i>
22 0	25.6	-	1604	0	0	-
22 1	Cedrol	1598	1606	7229	12776	Cedrol found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Candida Albicans</i> , <i>Staphylococcus Aureus</i> , <i>Metschnikowia Reukaufii</i> , <i>Debaryomyces Hansenii</i>
22 2	30.4	-	1607	13355	1585	-
22 3	30.4	-	1609	0	1310	-
22 4	Lauryl acetate	1607	1613	24313	21666	Lauryl acetate found in: 1. mVOC database / <i>Candida Albicans</i> , <i>Candida Glabrata</i> , <i>Candida Tropicalis</i>
22 5	30.6	-	1615	16585	16446	-
22 6	30.6	-	1616	1720	0	-
22 7	30.7	-	1617	3168	8898	-
22 8	30.7	-	1618	764	0	-
22 9	30.7	1613 / 1605	1619	16769	85384	-
23 0	30.8	-	1623	0	2941	-
23 1	30.9	-	1624	182035	84101	-

23 2	31	-	1628	3945	5657	-
23 3	31	-	1629	43857	52497	-
23 4	31	-	1630	5984	15290	-
23 5	31.1	-	1633	992	0	-
23 6	31.2	-	1637	39406	50816	-
23 7	31.3	-	1639	0	3356	-
23 8	31.4	-	1644	4336	103239	-
23 9	31.5	-	1647	69023	47107	-
24 0	31.5	-	1649	3020	2144	-
24 1	31.6	-	1650	3090	9347	-
24 2	31.6	-	1651	1445	4242	-
24 3	31.7	-	1653	633	869	-
24 4	31.7 ^b	1675 / 1643 / 1660	1655	3488	13108	-
24 5	Methyl jasmonate	1638	1656	8301	20794	Methyl jasmonate found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Lasiodiplodia Theobromae</i>
24 6	Cubenol	1659	1659	58343	291548	Cubenol found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Chondromyces Crocatus</i> , <i>Streptomyces Sp.</i> , <i>Streptomyces Caviscabies</i>
24 7	Tridecanoic acid / 31.9 / Cyclopentaneacetic acid, 3-oxo-2- pentyl-, methyl ester	1666 / 1649	1660	92194	2772	Tridecanoic acid found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Saccharomyces Cerevisiae</i> , <i>Bacillus Subtilis</i>

						Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester found in: 1. mVOC database / <i>Trichoderma Viride</i> , <i>Stropharia Rugosoannulata</i> , <i>Laccaria Bicolor</i>
24 8	32	-	1664	125428	132701	-
24 9	32	-	1665	10556	7593	-
25 0	32	-	1666	4535	8111	-
25 1	32	-	1667	344277	2579995	-
25 2	32.1	-	1668	481931	663591	-
25 3	32.1	-	1670	8789	35859	-
25 4	32.2	-	1674	2315223	2368069	-
25 5	32.3	-	1675	0	50205	-
25 6	32.3	-	1676	35171	0	-
25 7	32.4	-	1679	2558	5082	-
25 8	32.4	-	1680	8430	15682	-
25 9	32.4	-	1681	231731	0	-
26 0	32.5	-	1683	226064	229566	-
26 1	32.5	-	1684	3182	0	-
26 2	32.6	-	1688	147143	43110	-
26 3	32.7	-	1690	0	132723	-
26 4	2-Hexadecanol	1702	1692	52585	67827	2-Hexadecanol found in: 1. mVOC database / <i>Pleurotus</i> <i>Ostreatus</i>
26 5	32.8	-	1694	0	6726	-
26 6	32.9	-	1698	3643182	4258157	-

26 7	Pentadecane, 2,6,10,14- tetramethyl-	1690	1706	84643	95731	Pentadecane, 2,6,10,14- tetramethyl- found in: 1. mVOC database / <i>Pleurotus Ostreatus</i>
26 8	2-Hexadecanol	1702	1707	10590	19397	2-Hexadecanol found in: 1. mVOC database / <i>Streptomyces Thermocarboxydus, Trichoderma Harzianum</i>
26 9	33.2	-	1709	15766	28763	-
27 0	33.2	-	1710	0	19096	-
27 1	33.3	-	1711	223656	278522	-
27 2	33.4	-	1715	21127	16244	-
27 3	Pentadecanal-	1715	1716	0	12163	Pentadecanal- found in: 1. mVOC database / <i>Pediococcus Acidilactici, Erwinia Amylovora, Saccharomyces Cerevisiae</i>
27 4	33.5	-	1720	4867306	6503883	-
27 5	33.7	-	1729	18402	28767	-
27 6	33.8	-	1730	2624	9453	-
27 7	33.8	-	1731	111645	22634	-
27 8	33.9	-	1735	28134	33943	-
27 9	33.9	-	1736	5681	13461	-
28 0	34	-	1739	2068	11738	-
28 1	34	-	1740	68115	93575	-
28 2	10-Methyldodec- 2-en-4-olide	1758	1741	2502	0	10-Methyldodec-2-en-4-olide found in: 1. mVOC database / <i>Streptomyces Sp., Streptomyces Caviscabies</i>
28 3	34.1	-	1743	2721	12763	-

28 4	Heptadecane, 7-methyl-	1740	1745	247314	388085	Heptadecane, 7-methyl- found in: 1. mVOC database / <i>Cyanobacteria Sp.</i> , <i>Plectonema Notatum</i> , <i>Plectonema Sp.</i> , <i>Tolypothrix Distorta</i>
28 5	34.2	-	1748	28237	1930	-
28 6	34.3	-	1749	33023	8932	-
28 7	34.3	-	1750	0	924209	-
28 8	Tetradecanoic acid	1768	1751	77867	65345	Tridecanoic acid found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Saccharomyces Cerevisiae</i> , <i>Bacillus Subtilis</i>
28 9	34.4 ^b	-	1752	106130	7771	-
29 0	34.5	-	1754	0	73219	-
29 1	2-methyl-heptadecane ^b	1765	1755	160429	340221	Discussed in the main text
29 2	34.5	-	1759	259382	348941	-
29 3	34.6	-	1760	47220	29523	-
29 4	34.7	-	1764	48675	62577	-
29 5	34.8	-	1768	0	14616	-
29 6	34.8	-	1769	4988	1075	-
29 7	34.8	-	1770	8358	39086	-
29 8	34.9	-	1772	361851	370293	-
29 9	34.9	-	1773	0	2085	-
30 0	35	-	1776	103853	495463	-
30 1	35.1	-	1780	92628	0	-

30 2	35.2	-	1782	0	1501	-
30 3	35.2	-	1783	29421	16641	-
30 4	35.2	1788	1786	0	2917	-
30 5	35.3	-	1789	135470	0	-
30 6	35.3 / 35.4	-	1790	1972983	1625709	-
30 7	35.5	-	1795	14463	16619	-
30 8	Tetradecanoic acid, ethyl ester	1793	1796	47338	21403	Tetradecanoic acid, ethyl ester found in: 1. mVOC database / <i>Escherichia Coli</i> , <i>Bacillus Wiedmannii</i> , <i>Lentilactobacillus Buchneri</i> , <i>Lacticaseibacillus Paracasei</i>
30 9	35.6	-	1797	327	5745	-
31 0	35.6	1798	1800	1092807	1343009	-
31 1	35.8	1821	1805	40935	80742	-
31 2	35.9	-	1810	88737	49068	-
31 3	36	-	1815	15389	25035	-
31 4	36	-	1816	46229	109523	-
31 5	36.1	-	1819	25559	105687	-
31 6	36.1	1823	1820	22366	17287	-
31 7	E-9-Hexadecenal	1804	1821	109737	47192	E-9-Hexadecenal found in: 1. mVOC database / <i>Pseudomonas Sp.</i>
31 8	36.2	1835	1822	0	23107	-
31 9	Isopropyl myristate	1825	1829	3003685	1552980	Isopropyl myristate found in: 1. mVOC database / <i>Candida Albicans</i> , <i>Candida Glabrata</i> , <i>Tuber Borchii</i> , <i>Lentilactobacillus Buchneri</i>

320	36.4	-	1830	20397	15575	-
321	2,4-Diphenyl-4-methyl-2(E)-pentene	1836	1835	2017094	1915240	2,4-Diphenyl-4-methyl-2(E)-pentene found in: 1. mVOC database / <i>Pleurotus Cystidiosus</i>
322	36.5	-	1836	17119	44236	-
323	36.7	-	1843	342106	639558	-
324	36.7	-	1844	0	74640	-
325	36.7	-	1845	65927	136555	-
326	36.8	-	1847	1735	45980	-
327	36.9	-	1848	446148	565371	-
328	36.9	-	1852	186242	223745	-
329	37	-	1854	2909	3022	-
330	37	-	1856	180592	61013	-
331	37.1	-	1858	715917	1584306	-
332	37.1	-	1859	19109	75602	-
333	37.2	-	1864	433128	441007	-
334	37.3	-	1866	5426	91488	-
335	37.4	-	1872	425775	432899	-
336	37.5	-	1876	12349	16390	-
337	37.7	-	1881	39263	5266	-
338	37.7 / 1-Hexadecanol	1880	1882	100359	275648	1-Hexadecanol found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Escherichia Coli</i> , <i>Bacillus Velezensis</i> , <i>Bacillus Simplex</i> , <i>Bacillus Weiherstephanensis</i>

33 9	37.7	1885	1883	0	1091	-
34 0	37.7	-	1884	1126	0	-
34 1	Heptachlor	1887	1887	0	30115	Heptachlor found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Aspergillus Flavus</i>
34 2	37.8	-	1888	9018	2335	-
34 3	37.8 / 37.9	-	1889	58994	40546	-
34 4	38	-	1893	58776	120521	-
34 5	38	-	1894	229092	291461	-
34 6	Ethyl pentadecanoate / heptadecanol ^b	1894 / 1909	1897	387187	58473	Discussed in the main text
34 7	38.1	-	1898	7631	0	-
34 8	2,6,10,15- tetramethyl- heptadecane ^b	1889	1901	279991	667832	Discussed in the main text
34 9	1-Nonadecene	1893	1905	156950	267652	1-Nonadecene found in: 1. mVOC database / <i>Tuber Panniferum, Cyberlindnera Fabianii, Lactobacillus Plantarum</i>
35 0	38.3	-	1909	0	212939	-
35 1	38.4	-	1912	458587	386497	-
35 2	38.5	-	1914	0	49103	-
35 3	38.6	-	1918	21334	34114	-
35 4	38.6	-	1919	248986	255298	-
35 5	38.7	-	1924	1444	0	-
35 6	38.7	-	1925	106119	147765	-
35 7	38.8	1923	1929	5227	11295	-

35 8	38.8 / 38.9	-	1930	100488	85508	-
35 9	Palmitoleic acid	1951	1934	26946	12993	Palmitoleic acid found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Streptomyces Sp.</i>
36 0	Aldrin	1955	1935	40588	83520	Aldrin found in: 1. KEGG COMPOUND Database 2. mVOC database / <i>Pleurotus Ostreatus, Saccharomyces Cerevisiae</i>
36 1	39.1	-	1939	2161	0	-
36 2	Nonadecane, 9-methyl-	1936	1942	1292025	1178847	Nonadecane, 9-methyl- found in: 1. mVOC database / <i>Bacillus Subtilis</i>
36 3	39.2	-	1945	0	20700	-
36 4	39.3	-	1947	4422	9939	-
36 5	39.3	-	1948	272066	352847	-
36 6	39.4	-	1952	126919	279531	-
36 7	39.4	1936	1953	138767	99103	-
36 8	39.6	-	1960	0	2129	-
36 9	39.7	-	1964	4914	2888	-
37 0	39.7	-	1965	108733	165414	-
37 1	39.8	-	1967	51815	75387	-
37 2	39.8	-	1968	124279	99227	-
37 3	39.9	-	1972	242297	343879	-
37 4	40.0 / 40.1	-	1980	99322	101819	-
37 5	40.1	-	1983	368	2581	-

37 6	40.1	-	1984	5768	5699	-
37 7	40.2	-	1986	67305	34694	-
37 8	40.2	-	1987	8027	1107	-
37 9	40.3	-	1989	519	0	-
38 0	40.3	-	1990	149552	159934	-
38 1	40.4	-	1996	0	14783	-
38 2	40.5	-	1997	335792	223821	-
38 3	39.9 / 39.6	-	2002	8610	7645	-
38 4	39.4 / 39.2	-	2003	7098	9449	-

^a Combined feature containing peak or compounds with the “/” sign.

^b Feature proposed as the high stress markers discussed in the main text.