

Supplementary Materials

for the article

Volatile organic biogenic compounds (VBOCs) with two dimensional gas chromatography-time of flight mass spectrometry (GC \times GC-TOFMS): Sampling methods, VBOC complexity, and chromatographic retention data.

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Table S1. First dimension retention index (I_1) and second dimension retention ratio (R_2) for the 21 standard compounds (boldface) and for 417 other tentatively identified compounds in four sample chromatograms. Isomers that could not be differentiated are *italicized*.

compound	CAS Number	I_1	R_2
alkanes, alkenes, alkynes, arenes			
butane, 2-methyl-	78-78-4	482	0.980
pentane	109-66-0	500	1.001
cyclopropane, 1,2-dimethyl-, cis-	930-18-7	507	1.027
isoprene	78-79-5	510	1.090
1-butene, 3-methyl-	563-45-1	517	1.019
cyclopropane, 1,1-dimethyl-	1630-94-0	520	1.031
2-pentene	109-68-2	527	1.025
1,3-cyclopentadiene	542-92-7	542	1.162
cyclopropane, ethyl-	1191-96-4	565	1.022
pentane, 2-methyl-	107-83-5	567	0.989
pentane, 3-methyl-	96-14-0	582	0.999
cyclopropane, 1-ethyl-2-methyl-, cis-	19781-68-1	590	1.021
hexane	110-54-3	600	0.996
cyclobutane, 1,2-bis(methylene)-	14296-80-1	602	1.145
isopropenylcyclopropane	4663-22-3	614	1.077
hexane, 2-methyl-	591-76-4	633	0.992
cyclopentane, methyl-	96-37-7	633	1.018
pentane, 2,4-dimethyl-	108-08-7	635	0.999
1,4-hexadiene, (Z)-	7318-67-4	656	1.065
1-hexene, 4,5-dimethyl-	16106-59-5	660	1.007
cyclohexane	110-82-7	667	1.035
benzene	71-43-2	673	1.303
hexane, 3-methyl-	589-34-4	677	1.004
heptanes	142-82-5	700	1.002
hexane, 2,2-dimethyl-	590-73-8	726	1.001
cyclohexane, methyl-	108-87-2	731	1.036
heptane, 2-methyl-	592-27-8	733	1.002
hexane, 2,4-dimethyl-	589-43-5	738	1.003
cyclopentane, ethyl-	1640-89-7	741	1.037
hexane, 2,5-dimethyl-	592-13-2	767	1.006
toluene	108-88-3	782	1.264
pentane, 3-ethyl-2,2-dimethyl-	16747-32-3	787	1.000
cyclohexane, 1,2-dimethyl-, cis-	2207-01-4	790	1.028
2-octene, (E)-	13389-42-9	792	1.021
octane	111-65-9	800	1.007
heptane, 2,5-dimethyl-	2216-30-0	839	0.999
cyclohexane, ethyl-	1678-91-7	845	1.040
hexane, 3-ethyl-	619-99-8	867	0.997
heptane, 3-ethyl-	15869-80-4	876	0.996
ethylbenzene	100-41-4	885	1.221
<i>m</i> -xylene + <i>p</i> -xylene	108-38-3; 106-42-3	891	1.221
cyclooctane, methyl-	1502-38-1	894	1.021

compound	CAS Number	<i>I</i> ₁	<i>R</i> ₂
nonane	111-84-2	900	0.992
cis-1-ethyl-3-methyl-cyclohexane	19489-10-2	903	1.020
styrene	100-42-5	913	1.350
<i>o</i> -xylene	95-47-6	917	1.249
3a,4,5,6,7,7a-hexahydro-4,7-methanoindene	4488-57-7	937	1.088
nonane, 3-methyl-	5911-04-6	940	0.981
cumene	98-82-8	943	1.184
heptane, 3-ethyl-2-methyl-	14676-29-0	950	0.985
3-octen-5-yne, 2,7-dimethyl-, (E)-	55956-33-7	953	1.069
3-octen-5-yne, 2,7-dimethyl-, (Z)-	28935-76-4	953	1.052
nonane, 2-methyl-	871-83-0	967	0.980
benzene, propyl-	103-65-1	973	1.190
dehydrosabinene	36262-09-6	977	1.110
benzene, 1-ethyl-2-methyl-	611-14-3	980	1.188
benzene, 1-ethyl-4-methyl-	622-96-8	983	1.174
1-decene	872-05-9	993	1.010
benzene, 1,3,5-trimethyl-	108-67-8	993	1.198
decane	124-18-5	1000	0.999
ethanol, 2-(2-ethoxyethoxy)-	111-90-0	1000	1.820
benzene, 1-ethyl-3-methyl-	620-14-4	1003	1.214
2,6-dimethyl-1,3,5,7-octatetraene, E,E- (or an isomer))	460-01-5	1007	1.141
2,6-dimethyl-1,3,5,7-octatetraene, E,E - (or an isomer)	460-01-5	1020	1.152
benzene, 1,2,4-trimethyl-	95-63-6	1020	1.230
benzene, 2-propenyl-	300-57-2	1020	1.321
decane, 4-methyl-	2847-72-5	1023	0.981
nonane, 2,6-dimethyl-	17302-28-2	1023	0.984
benzene, 1-ethenyl-3-methyl-	100-80-1	1023	1.321
benzene, butyl-	104-51-8	1027	1.176
benzene, 1-methyl-2-propyl-	1074-17-5	1030	1.184
benzene, 1-methyl-4-(1-methylethethyl)- (or an isomer)	1195-32-0	1030	1.227
cyclohexene, 3-methyl-6-(1-methylethyl)-	5256-65-5	1040	1.074
p-cymene	99-87-6	1043	1.197
cyclohexane, propyl-	1678-92-8	1047	1.038
cyclohexane, (1-methylpropyl)-	7058-01-7	1047	1.044
benzene, 1,2,3-trimethyl-	526-73-8	1053	1.305
benzene, 1-ethyl-3,5-dimethyl-	934-74-7	1060	1.231
2,6-octadiene, 2,6-dimethyl-	2792-39-4	1063	1.340
benzene, 1,3-diethyl-	141-93-5	1067	1.222
indane	496-11-7	1067	1.371
decane, 3-methyl-	13151-34-3	1070	0.995
benzene, 1-methyl-3-propyl-	1074-43-7	1070	1.228
benzene, 1,4-diethyl-	105-05-5	1077	1.232
benzene, 2-ethyl-1,4-dimethyl-	1758-88-9	1080	1.245
benzene, 1-propynyl-	673-32-5	1083	1.597
benzene, 1-methyl-4-propyl-	1074-55-1	1093	1.273
undecane	1120-21-4	1100	1.001
benzene, 1-ethyl-2,4-dimethyl-	874-41-9	1103	1.281
benzene, (2-methyl-1-propenyl)-	768-49-0	1106	1.379
benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	1109	1.294
benzene, 1-methyl-4-(1-methylethethyl)- (or an isomer)	1195-32-0	1115	1.392
undecane, 2,6-dimethyl-	17301-23-4	1120	0.999
benzene, 1-methyl-4-(2-propenyl)-	3333-13-9	1126	1.419
decane, 2-methyl-	6975-98-0	1129	0.992
decane, 2,6,6-trimethyl-	62108-24-1	1131	0.989
2,6-dimethyl-1,3,5,7-octatetraene, E,E- (or an isomer)	460-01-5	1135	1.307
benzene, 4-ethyl-1,2-dimethyl-	934-80-5	1138	1.344
<i>undecane, 3-methyl- (or an isomer)</i>	1002-43-3	1144	0.993

compound	CAS Number	<i>I</i> ₁	<i>R</i> ₂
benzene, 1,3-diethenyl-	108-57-6	1147	1.593
naphthalene, decahydro-2-methyl-	2958-76-1	1150	1.106
cyclohexane, pentyl-	4292-92-6	1153	1.054
benzene, 1,2,4,5-tetramethyl-	95-93-2	1154	1.347
benzene, 1,2,3,5-tetramethyl-	527-53-7	1157	1.358
1,2,3,4,5,8-hexahydronaphthalene	36231-13-7	1159	1.330
benzene, 2-ethyl-1,3-dimethyl-	2870-04-4	1159	1.355
benzene, 1,2-diethenyl-	135-01-3	1162	1.618
undecane, 2-methyl-	7045-71-8	1165	0.994
benzene, 1-methyl-4-(1-methylpropyl)-	1595-16-0	1165	1.265
2,6-dimethyl-1,3,5,7-octatetraene, <i>E,E</i> (or an isomer)	460-01-5	1165	1.340
decane, 2,9-dimethyl-	1002-17-1	1166	0.998
1-methyldecahydronaphthalene	2958-75-0	1168	1.125
bicyclo[3.2.1]oct-2-ene, 3-methyl-4-methylene-	49826-53-1	1168	1.345
undecane, 3-methyl- (or an isomer)	1002-43-3	1174	0.997
benzene, 1-methyl-4-(2-methylpropyl)-	5161-04-6	1174	1.269
1h-indene, 2,3-dihydro-5-methyl-	874-35-1	1177	1.433
benzene, pentyl-	538-68-1	1180	1.273
benzene, 1-methyl-2-(2-propenyl)-	1587-04-8	1191	1.460
1h-indene, 2,3-dihydro-4-methyl-	824-22-6	1191	1.464
1-dodecene	112-41-4	1194	1.036
benzene, 1,3-diethyl-5-methyl-	2050-24-0	1194	1.291
benzene, 1-methyl-2-(1-methylethyl)-	527-84-4	1197	1.409
naphthalene, 1,2-dihydro-	447-53-0	1197	1.639
dodecane	112-40-3	1200	1.003
cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	1213	1.042
decane, 2,6,7-trimethyl-	62108-25-2	1216	0.990
1h-indene, 2,3-dihydro-1,6-dimethyl-	17059-48-2	1221	1.368
1h-indene, 2,3-dihydro-1,1-dimethyl-	4912-92-9	1224	1.384
benzene, 1,3-dimethyl-5-(1-methylethyl)-	4706-90-5	1232	1.345
1h-indene, 2,3-dihydro-1,3-dimethyl-	4175-53-5	1237	1.416
undecane, 5-ethyl-	17453-94-0	1242	0.990
benzene, 1-ethyl-4-(1-methylethyl)-	4218-48-8	1242	1.359
naphthalene	91-20-3	1242	2.010
benzene, 1-methyl-3-(1-methyl-2-propenyl)-	52161-57-6	1250	1.441
cyclohexane, hexyl-	4292-75-5	1258	1.059
decane, 2,3,4-trimethyl-	62238-15-7	1261	0.990
dodecane, 3-methyl-	17312-57-1	1274	0.993
benzene, (1,3-dimethylbutyl)-	19219-84-2	1295	1.303
7-methyl-1,2,3,5,8,8a-hexahydronaphthalene	107914-88-5	1295	1.370
1h-indene, 2,3-dihydro-4,7-dimethyl-	6682-71-9	1295	1.473
tridecane	629-50-5	1300	0.999
1h-indene, 1,1-dimethyl-	18636-55-0	1305	1.632
naphthalene, 1,2,3,4-tetrahydro-6-methyl-	1680-51-9	1310	1.508
naphthalene, 1,2,3,4-tetrahydro-5-methyl-	2809-64-5	1310	1.509
1-decene, 8-methyl-	61142-79-8	1347	1.645
2,4,6-trimethyl-1,3,6-heptatriene	24648-33-7	1355	1.427
naphthalene, 2-methyl-	91-57-6	1360	1.992
naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	4175-54-6	1365	1.466
tridecane, 3-methyl-	6418-41-3	1373	0.993
naphthalene, 1-methyl-	90-12-0	1378	2.062
benzene, (2,2-dimethylbutyl)-	28080-86-6	1385	1.959
3-tetradecene, (<i>Z</i>)-	41446-67-7	1392	1.037
tetradecane	629-59-4	1400	1.000
biphenyl	92-52-4	1429	2.161
naphthalene, 2-ethyl-	939-27-5	1456	1.964
1,6,10-dodecatriene, 7,11-dimethyl-3-methylene-, (<i>E</i>)-	18794-84-8	1463	1.189

compound	CAS Number	I₁	R₂
naphthalene, 2,3-dimethyl-	581-40-8	1476	1.958
naphthalene, 1,4-dimethyl-	571-58-4	1490	2.035
pentadecane	629-62-9	1500	1.001
1,8-cyclopentadecadiyne	4722-42-3	1500	1.316
c16 isomer	n/a	1507	0.950
diphenylmethane	101-81-5	1536	2.108
naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	1985-59-7	1540	2.679
naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylethyl)-, (1s-cis)-	483-77-2	1564	1.395
α-calacorene	21391-99-1	1590	1.498
hexadecane	544-76-3	1600	1.002
c17 isomer	n/a	1654	0.973
heptadecane	629-78-7	1700	0.994
heptadecane, 2,6-dimethyl-	54105-67-8	1712	0.956
heptadecane, 2-methyl-	1560-89-0	1763	0.990
1-nonadecene	18435-45-5	1793	1.051
octadecane	593-45-3	1800	1.004
c19 isomer	n/a	1814	0.968
hexadecane, 2,6,10,14-tetramethyl-	638-36-8	1814	0.968
octadecane, 2-methyl-	1560-88-9	1863	0.989
nonadecane	629-92-5	1900	1.000

alcohols, ketones, aldehydes, furans

2-propenal	107-02-8	492	1.661
isopropyl alcohol	67-63-0	492	2.169
propanal	123-38-6	495	1.445
acetone	67-64-1	498	1.528
furan	110-00-9	505	1.377
propanal, 2-methyl-	78-84-2	560	1.261
methacrolein	78-85-3	571	1.433
2,3-dihydrofuran	1191-99-7	580	1.294
2,3-butanedione	431-03-8	590	1.668
butanal	123-72-8	593	1.350
methyl vinyl ketone	78-94-4	593	1.590
2-butanone	78-93-3	600	1.391
furan, 2-methyl-	534-22-5	609	1.261
furan, 3-methyl-	930-27-8	618	1.308
2-butenal, (E)-	123-73-9	659	1.648
butanal, 3-methyl-	590-86-3	660	1.259
butanal, 2-methyl-	96-17-3	670	1.229
1-penten-3-ol	616-25-1	679	1.855
2-pentanone	107-87-9	690	1.323
1-penten-3-one	1629-58-9	691	1.410
pentanal	110-62-3	700	1.292
cyclopentanol	96-41-3	700	1.305
methyl isobutyl ketone	108-10-1	749	1.255
3-pentanone, 2-methyl-	565-69-5	756	1.228
3-hexanone	589-38-8	756	1.209
butanedial	638-37-9	777	2.804
2-butenal, 3-methyl-	107-86-8	795	1.555
3-hexenal, (Z)-	6789-80-6	800	1.361
hexanal	66-25-1	803	1.271
3-penten-2-one, 4-methyl-	141-79-7	809	1.352
3-furaldehyde	498-60-2	842	2.284
3-hexen-1-ol, (Z)-	928-96-1	856	1.732
2-pentanone, 3-methyl-	565-61-7	862	2.182
2-hexenal, (E)-	6728-26-3	864	1.384

compound	CAS Number	I₁	R₂
1-hexanol	111-27-3	865	1.575
5-hexen-2-one, 5-methyl-3-methylene-	51756-18-4	891	1.167
3-heptanone	106-35-4	891	1.215
2-heptanone	110-43-0	897	1.240
2-heptanol	543-49-7	897	1.374
heptanal	111-71-7	907	1.231
cyclohexanone	108-94-1	913	1.476
2-butene-1,4-diol	110-64-5	927	2.135
butyrolactone	96-48-0	927	2.642
2(5h)-furanone	497-23-4	927	3.469
2,5-furandione, dihydro-3-methylene-	2170-03-8	950	2.764
2-heptanone, 6-methyl-	928-68-7	963	1.205
hexanal, 2-ethyl-	123-05-7	967	1.138
1-heptanol	111-70-6	967	1.463
2-heptenal, (Z)-	57266-86-1	970	1.330
1-octen-3-ol	3391-86-4	980	1.413
1-octen-3-one	4312-99-6	987	1.240
3-heptanone, 5-methyl-	541-85-5	990	1.186
5-hepten-2-one, 6-methyl-	110-93-0	993	1.277
2-octanone	111-13-7	997	1.210
3-methyl-3-cyclohexen-1-one	31883-98-4	1007	1.502
octanal	124-13-0	1010	1.206
1-hexanol, 2-ethyl-	104-76-7	1027	1.417
1-octanol	111-87-5	1067	1.552
2-octenal, (E)-	2548-87-0	1073	1.414
2,6-octadienal, 3,7-dimethyl-, (E)-	141-27-5	1077	1.058
7-octen-2-ol, 2,6-dimethyl-	18479-58-8	1077	1.363
2(3h)-furanone, 5-ethyldihydro-	695-06-7	1077	2.315
2-nonanone	821-55-6	1100	1.302
2-nonanol	628-99-9	1100	1.436
nonanal	124-19-6	1112	1.297
1,7-octadien-3-one, 2-methyl-6-methylene-	41702-60-7	1153	1.502
4-acetyl-1-methylcyclohexene	6090-09-1	1159	1.600
1,5,7-octatrien-3-ol, 2,6-dimethyl-	29414-56-0	1162	1.939
1-nonanol	143-08-8	1171	1.639
2,6-octadienal, 3,7-dimethyl-	5392-40-5	1203	1.754
decanal	112-31-2	1216	1.313
ethanone, 1-(4-methylphenyl)-	122-00-9	1226	2.119
2(3h)-furanone, 5-butyldihydro-	104-50-7	1289	2.446
2-undecanone	112-12-9	1305	1.330
undecanal	112-44-7	1318	1.332
1-undecanol	112-42-5	1375	1.647
dodecanal	112-54-9	1422	1.333
5,9-undecadien-2-one, 6,10-dimethyl-, (E)-	3796-70-1	1466	1.504
tetradecanal	124-25-4	1524	1.323
pentadecanal	2765-11-9	1628	1.316
hexadecanal	629-80-1	1728	1.310
2-butanol, 3-(2,2-dimethylpropoxy)-	74793-66-1	1935	2.309

ethers, carboxylic acids, esters

ethene, ethoxy-	109-92-2	505	1.135
acetic acid, methyl ester	79-20-9	538	1.356
ethyl acetate	141-78-6	619	1.277
formic acid, propyl ester	110-74-7	625	1.343
2-propenoic acid, 2-methyl-, methyl ester	80-62-6	715	1.290
formic acid, butyl ester	592-84-7	728	1.291
butanoic acid, 3-methyl-, methyl ester	556-24-1	779	1.203

compound	CAS Number	<i>I</i> ₁	<i>R</i> ₂
acetic acid, butyl ester	123-86-4	815	1.216
2-pentanol, acetate	626-38-0	850	1.167
2-butenoic acid, 3-methyl-, methyl ester	924-50-5	856	1.301
2-propen-1-ol, 2-methyl-, acetate	820-71-3	859	2.216
2-butenoic acid, 2-methyl-, methyl ester	41725-90-0	874	1.298
1-butanol, 3-methyl-, acetate	123-92-2	879	1.176
ethanol, 2-butoxy-	111-76-2	907	1.599
acetic acid, pentyl ester	628-63-7	913	1.180
2-buten-1-ol, 3-methyl-, acetate	1191-16-8	920	1.269
hexanoic acid	142-62-1	957	3.423
2-pentenoic acid, 3-methyl-, methyl ester	50652-79-4	960	1.253
3-hexen-1-ol, acetate, (Z)-	3681-71-8	1007	1.219
acetic acid, hexyl ester	142-92-7	1010	1.160
hexanoic acid, 4-methylene-, methyl ester	73805-48-8	1027	1.254
oxalic acid, bis(isobutyl) ester	n/a	1030	0.976
2-butoxyethyl acetate	112-07-2	1080	1.373
acetic acid, octyl ester	112-14-1	1211	1.253
nonanoic acid	112-05-0	1255	4.011
acetic acid, nonyl ester	143-13-5	1310	1.261
acetic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	92618-89-8	1318	1.349
2-decanoic acid, methyl ester, (E)-	7367-85-3	1325	1.341
2,6-octadienoic acid, 3,7-dimethyl-, methyl ester	2349-14-6	1332	1.459
n-decanoic acid	334-48-5	1355	3.870
2,6-octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-	141-12-8	1365	1.418
propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl ester	74367-33-2	1390	1.797
propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	1402	1.663
2-propenoic acid, 3-phenyl-, methyl ester	103-26-4	1422	2.464
dodecanoic acid	143-07-7	1555	3.597
propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	1623	1.271
octane, 1,1'-oxybis-	629-82-3	1663	1.067
Z-11-tetradecenoic acid	79039-46-6	1795	1.729
n-hexadecanoic acid	57-10-3	1971	1.654

oxygenated aromatics

oxepine, 2,7-dimethyl-	1487-99-6	947	1.237
benzaldehyde	100-52-7	987	1.760
benzenacetraldehyde, α -methyl-	93-53-8	1030	1.182
3-hydroxyphenylacetylene	10401-11-3	1030	1.623
benzenacetraldehyde	122-78-1	1063	2.013
acetophenone	98-86-2	1100	2.059
benzaldehyde, 3-methyl-	620-23-5	1103	1.967
benzenemethanol, α,α -dimethyl-	617-94-7	1106	2.304
benzoic acid, methyl ester	93-58-3	1126	1.853
phenylethyl alcohol	60-12-8	1135	3.141
acetic acid, phenylmethyl ester	140-11-4	1182	1.984
benzaldehyde, 4-ethyl-	4748-78-1	1200	1.961
benzenemethanol, α,α ,4-trimethyl-	1197-01-9	1211	2.278
benzaldehyde, 2,5-dimethyl-	5779-94-2	1218	2.024
cinnamaldehyde, (E)-	14371-10-9	1221	2.351
phenol, 2,4,6-trimethyl-	527-60-6	1232	3.028
methyl salicylate	119-36-8	1237	2.087
benzoic acid, 3-methyl-, methyl ester	99-36-5	1239	1.883
2-propenal, 3-phenyl-	104-55-2	1239	2.437
benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-	1076-56-8	1247	1.424

compound	CAS Number	I₁	R₂
benzoic acid, 4-methyl-, methyl ester	99-75-2	1250	1.908
ethanol, 2-phenoxy-	122-99-6	1250	4.085
benzenepropanol	122-97-4	1253	3.224
acetic acid, 2-phenylethyl ester	103-45-7	1276	1.972
propiophenone, 2'-methyl-	2040-14-4	1323	2.009
3-penten-2-one, 5-phenyl-	10521-97-8	1363	2.176
benzoic acid, 4-acetyl-, methyl ester	3609-53-8	1521	3.099
diethyl phthalate	84-66-2	1623	2.645
benzophenone	119-61-9	1688	3.016
1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	1896	2.507

monoterpenes

bicyclo[2.2.1]hept-2-ene, 1,7,7-trimethyl-	464-17-5	923	1.044
thujene	58037-87-9	940	1.052
α-pinene	80-56-8	957	1.021
camphene	79-92-5	973	1.084
sabinene	3387-41-5	990	1.080
myrcene	123-35-3	993	1.145
β-pinene	127-91-3	1000	1.065
<i>α-phellandrene isomer</i>	n/a	1020	1.105
Δ³-carene	13466-78-9	1023	1.111
cyclohexene, 4-methyl-3-(1-methylethylidene)-	99805-90-0	1030	1.110
<i>γ-terpinene (or an isomer)</i>	99-85-4	1033	1.116
limonene	138-86-3	1047	1.131
α-phellandrene	99-83-2	1050	1.149
<i>γ-terpinene (or an isomer)</i>	99-85-4	1070	1.156
terpinolene	586-62-9	1106	1.191

oxygenated monoterpenes

eucalyptol	470-82-6	1050	1.144
<i>d-verbenol (or an isomer)</i>	473-67-6	1103	1.672
linalool	78-70-6	1106	1.497
<i>d-verbenol (or an isomer)</i>	473-67-6	1115	1.545
α-pinene epoxide	1686-14-2	1138	1.331
2-cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, <i>trans</i> - (or an isomer)	7212-40-0	1144	1.715
2-cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, <i>trans</i> - (or an isomer)	7212-40-0	1159	1.803
limonene oxide, cis-	4680-24-4	1162	1.373
cis-verbenol	18881-04-4	1171	1.752
<i>d-verbenol (or an isomer)</i>	473-67-6	1176	1.806
bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, (1 α ,3 α ,5 α)-	3310-02-9	1177	1.870
bicyclo[3.1.1]heptan-3-ol, 6,6-dimethyl-2-methylene-, [1s-(1 α ,3 α ,5 α)]-	547-61-5	1179	1.766
(1R)-(+)-nopinone	38651-65-9	1182	1.696
menthone	10458-14-7	1191	1.380
camphor	76-22-2	1191	1.517
menthol	1490-04-6	1203	1.611
borneol	464-45-9	1203	1.842
bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-	18358-53-7	1205	1.485
2(10)-pinen-3-one, (\pm)-	30460-92-5	1205	1.597
4-terpinenol	562-74-3	1208	1.553
bicyclo[3.3.0]oct-2-en-7-one, 6-methyl-	n/a	1208	1.919
cyclohexanol, 2-methylene-5-(1-methylethenyl)-	35907-10-9	1213	2.071
pinocamphone	547-60-4	1218	1.536

compound	CAS Number	I₁	R₂
terpineol	98-55-5	1221	1.720
estragole	140-67-0	1224	1.688
myrtenol	515-00-4	1226	2.038
cryptone	500-02-7	1232	1.807
myrtanal	4764-14-1	1234	1.547
myrtenal	564-94-3	1237	1.669
cis-carveol	1197-06-4	1242	2.090
fenchyl acetate	13851-11-1	1250	1.269
1-verbeneone	1196-01-6	1261	1.835
carvone	99-49-0	1279	1.801
3-carvomenthenone	89-81-6	1297	1.768
α-thujenal	57129-54-1	1303	1.856
bicyclo[3.1.0]hex-3-en-2-ol, 2-methyl-5-(1-methylethyl)-, (1 α ,2 α ,5 α)-	97631-68-0	1315	1.410
trans-pinocarvyl acetate	1686-15-3	1327	1.436
myrtenyl acetate	1079-01-2	1350	1.465
<u>sesquiterpenes</u>			
α-cubebene	17699-14-8	1383	1.117
α-longipinene	5989-08-02	1405	1.147
copaene	3856-25-5	1417	1.121
β-cubebene (or an isomer)	13744-15-5	1427	1.166
cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethyl)-	110823-68-2	1429	1.213
β-bourbonene	5208-59-3	1432	1.159
longicyclene	1137-12-8	1434	1.165
isoledene	n/a	1446	1.182
δ-elemene	20307-84-0	1451	1.173
isocaryophyllene	118-65-0	1454	1.208
β-patchoulene	514-51-2	1456	1.219
cis-α-bisabolene	29837-07-8	1461	1.201
aromadendrene isomer	n/a	1466	1.211
longifolene	475-20-7	1468	1.222
α-cedrene	469-61-4	1471	1.230
caryophyllene	87-44-5	1473	1.245
(Z,Z)- α -farnesene	n/a	1478	1.209
aromadendrene	489-39-4	1493	1.224
humulene	6753-98-6	1510	1.244
α-farnesene	502-61-4	1514	1.232
germacrene D (or an isomer)	23986-74-5	1519	1.144
α-murolene	31983-22-9	1519	1.254
β-cubebene (or an isomer)	13744-15-5	1524	1.149
(Z)-α-farnesene	28973-97-9	1524	1.270
α-amorphene	483-75-0	1536	1.263
(Z,E)-α-farnesene	26560-14-5	1538	1.251
calarene	17334-55-3	1543	1.295
clove	469-92-1	1545	1.295
δ-cadinene	483-76-1	1555	1.276
germacrene D (or an isomer)	23986-74-5	1557	1.298
santalene	512-61-85989	1559	1.249
naphthalene, 1,2,3,4,4 α ,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-	16728-99-7	1574	1.312
<u>oxygenated sesquiterpenes</u>			
longipinocarvone (or an isomer)	65556-52-7	1637	1.704
caryophyllene oxide (or an isomer)	1139-30-6	1650	1.546
caryophyllene oxide (or an isomer)	1139-30-6	1655	1.567
germacrone	6902-91-6	1655	1.703

compound	CAS Number	I₁	R₂
<i>longipinocarvone (or an isomer)</i>	65556-52-7	1660	1.717
<i>caryophyllene oxide (or an isomer)</i>	1139-30-6	1668	1.579
humulene epoxide 2	19888-34-7	1683	1.611
tetracyclo[6.3.2.0(2,5).0(1,8)]tridecan-9-ol, 4,4-dimethyl-	n/a	1695	2.086
<i>caryophyllene oxide (or an isomer)</i>	1139-30-6	1723	2.193
trans-Z- α -bisabolene epoxide	111536-37-9	1726	2.196
<u>S-,N-containing</u>			
dimethyl sulfide	75-18-3	520	1.238
carbon disulfide	75-15-0	540	1.161
disulfide, dimethyl	624-92-0	754	1.391
pentanenitrile, 4-methyl-	542-54-1	852	1.481
benzonitrile	100-47-0	1007	1.976
benzothiazole	95-16-9	1276	2.789
benzene, 2,4-diisocyanato-1-methyl-	584-84-9	1392	1.932
<u>Br-,Cl-,F-,I-containing</u>			
trichloromonofluoromethane	75-69-4	492	1.068
methylene chloride	75-09-2	530	1.836
ethane, 1,1,2-trichloro-1,2,2-trifluoro-	76-13-1	532	1.038
trichloromethane	67-66-3	616	1.711
ethane, 1,2-dichloro-	107-06-2	649	1.747
carbon tetrachloride	56-23-5	670	1.169
tetrachloroethylene	127-18-4	824	1.163
benzene, 1-chloro-4-(trifluoromethyl)-	98-56-6	867	1.241
benzene, 1,3-dichloro-	541-73-1	1040	1.491

Table S2. Positively identified compounds (**boldface**) and tentatively identified compounds in an ATD analysis of air from a field branch enclosure of *Calycolpus moritzianus* (see GCxGC-TOFMS chromatogram in Figure 3).

All peaks met the peak selection criteria.

Name	CAS	Formula	MW	Isotope Ave.	Retention Times	Peak Area
				(seconds)		
alkanes, alkenes, alkynes, arenes						
1 1-propene, 2-methyl-	115-11-7	C4H8	56.11	189.986 , 0.924		36799097
2 2-butene, (Z)-	590-18-1	C4H8	56.11	193.986 , 0.931		27134602
3 <u>isoprene</u>	78-79-5	C5H8	68.12	221.983 , 1.043		847807
4 cyclopentene	142-29-0	C5H8	68.12	233.982 , 1.076		852156
5 cyclopropane, ethyl-	1191-96-4	C5H10	70.14	209.984 , 0.977		49074671
6 1-butene, 3-methyl-	563-45-1	C5H10	70.14	217.983 , 1.003		4109525
7 benzene	71-43-2	C6H6	78.11	321.973 , 1.465		18373037
8 3-hexene, (Z)-	7642-09-3	C6H12	84.16	261.979 , 1.096		1040163
9 cyclopentane, methyl-	96-37-7	C6H12	84.16	285.976 , 1.142		365812
10 pentane, 2-methyl-	107-83-5	C6H14	86.18	237.981 , 1.023		2288853
11 hexane	110-54-3	C6H14	86.18	257.979 , 1.063		6699436
12 toluene	108-88-3	C7H8	92.14	453.96 , 1.267		20128124
13 heptane	142-82-5	C7H16	100.21	361.969 , 1.115		9668096
14 phenylethyne	536-74-3	C8H6	102.14	581.947 , 1.214		368840
15 styrene	100-42-5	C8H8	104.15	593.946 , 1.188		1973155
16 p-xylene	106-42-3	C8H10	106.17	573.948 , 1.142		3252420
17 o-xylene	95-47-6	C8H10	106.17	597.945 , 1.148		895463
18 1-octene	111-66-0	C8H16	112.22	477.957 , 1.063		3481745
19 <i>cumene</i>	98-82-8	C9H12	120.20	629.942 , 1.109		175965
20 benzene, propyl-	103-65-1	C9H12	120.20	653.94 , 1.102		354299
21 benzene, 1-ethyl-3-methyl-	620-14-4	C9H12	120.20	661.939 , 1.102		1181386
22 <i>cumene</i>	98-82-8	C9H12	120.20	689.936 , 1.102		1391752
23 cyclohexene, 3,3,5-trimethyl-	503-45-7	C9H16	124.23	525.952 , 1.056		1142424
24 cyclohexene, 3,5,5-trimethyl-	933-12-0	C9H16	124.23	533.952 , 1.056		895838
25 nonane	111-84-2	C9H20	128.26	601.945 , 0.983		1483728
26 naphthalene	91-20-3	C10H8	128.17	829.922 , 1.327		697335
27 benzene, 1-methyl-4-(1-methylethenyl)-	1195-32-0	C10H12	132.21	761.929 , 1.115		1407256
28 dehydrosabinene	36262-09-6	C10H14	134.22	657.939 , 1.056		278413

29 <u>p-cymene</u>	99-87-6	C10H14	134.22	713.934 , 1.082	95797518
30 decane	124-18-5	C10H22	142.29	689.936 , 0.964	288480
31 cyclohexane, 2-ethenyl-1,1-dimethyl-3-methylene-	95452-08-7	C11H18	140.19	773.928 , 1.030	898062
32 octane, 2,5,6-trimethyl-	62016-14-2	C11H24	156.31	657.939 , 0.964	264784
33 nonane, 2,6-dimethyl-	17302-28-2	C11H24	156.31	705.934 , 0.957	332332
34 undecane	1120-21-4	C11H24	156.31	761.929 , 0.964	1457662
35 biphenyl	92-52-4	C12H10	154.21	941.911 , 1.320	315862
36 decane, 2,6,6-trimethyl-	62108-24-1	C13H28	184.37	717.933 , 0.970	169898
37 tridecane	629-50-5	C13H28	184.37	825.922 , 0.970	443979
38 pentadecane	629-62-9	C13H28	184.37	937.911 , 1.010	426133
39 tetradecane	629-59-4	C14H30	171.18	881.917 , 1.003	260856
40 naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	483-78-3	C15H18	198.31	1081.9 , 1.300	1334760
41 isolongifolene, 4,5,9,10-dehydro-	156747-45-4	C15H20	200.33	1017.9 , 1.208	424667
42 α -calacorene	21391-99-1	C15H20	200.33	1021.9 , 1.221	829668
43 β -calacorene	50277-34-4	C15H20	200.33	1033.9 , 1.228	214642
44 hexadecane	544-76-3	C16H34	226.45	985.906 , 1.023	553561

alcohols, ketones, aldehydes, furans

45 2-propenal	107-02-8	C3H4O	56.06	209.984 , 1.135	20359656
46 acetone	67-64-1	C3H6O	58.08	209.984 , 1.155	21292024
47 maleic anhydride	108-31-6	C4H2O3	98.06	553.95 , 1.624	1541282
48 furan	110-00-9	C4H4O	68.08	213.984 , 1.043	12440463
49 methacrolein	78-85-3	C4H6O	70.09	241.981 , 1.346	679330
50 butyrolactone	96-48-0	C4H6O2	86.09	617.943 , 1.643	336383
51 butanal	123-72-8	C4H8O	72.11	253.98 , 1.465	572117
52 furfural	98-01-1	C5H4O2	96.09	533.952 , 1.465	341221
53 furan, 2-methyl-	534-22-5	C5H6O	82.10	261.979 , 1.254	308239
54 2(5h)-furanone, 5,5-dimethyl-	20019-64-1	C6H8O2	112.13	653.94 , 1.353	299648
55 hexanal	66-25-1	C6H12O	100.16	489.956 , 1.234	3909328
56 3-hexen-1-ol, (Z)-	928-96-1	C6H12O	100.16	557.949 , 1.195	1007985
57 1-hepten-3-one	2918-13-0	C7H12O	112.17	669.938 , 1.109	1775949
58 3-heptanone	106-35-4	C7H14O	114.19	585.946 , 1.135	570008
59 2-heptanone	110-43-0	C7H14O	114.19	589.946 , 1.142	501120
60 heptanal	111-71-7	C7H14O	114.19	601.945 , 1.122	1396168

61 1-heptanol	111-70-6	C7H16O	116.20	665.938 , 1.082	489772
62 5-hepten-2-one, 6-methyl-	110-93-0	C8H14O	126.20	677.937 , 1.115	2138804
63 1-octen-3-ol	3391-86-4	C8H16O	128.22	673.938 , 1.082	2529927
64 octanal	124-13-0	C8H16O	128.22	693.936 , 1.076	2498704
65 1-hexanol, 2-ethyl-	104-76-7	C8H18O	130.23	709.934 , 1.082	13321398
66 1-octanol	111-87-5	C8H18O	130.23	741.931 , 1.082	1356268
67 cyclohexanone, 3,3,5-trimethyl-	873-94-9	C9H16O	140.23	725.932 , 1.135	195888
68 cyclohexanol, 3,3,5-trimethyl-, cis-	933-48-2	C9H18O	142.24	733.932 , 1.102	2373401
69 nonanal	124-19-6	C9H18O	142.24	765.928 , 1.109	3576722
70 decanal	112-31-2	C10H20O	156.27	829.922 , 1.109	2111323
71 undecanal	112-44-7	C11H22O	170.30	889.916 , 1.102	357045

ethers, carboxylic acids, esters

72 acetic acid	64-19-7	C2H4O2	60.05	245.98 , 1.478	8236772
73 isopropyl myristate	110-27-0	C17H34O2	270.46	1129.89 , 1.096	1179765

oxygenated aromatics

74 phenol	108-95-2	C6H6O	94.11	673.938 , 1.267	4152986
75 benzaldehyde	100-52-7	C7H6O	106.12	661.939 , 1.340	11046264
76 benzenecarboxylic acid	65-85-0	C7H6O2	122.12	801.925 , 1.287	360756
77 benzyl alcohol	100-51-6	C7H8O	108.14	717.933 , 1.333	445088
78 benzofuran	271-89-6	C8H6O	118.14	693.936 , 1.214	639071
79 1,2-benzenedicarboxylic acid	88-99-3	C8H6O4	166.13	905.914 , 1.459	4274294
80 acetophenone	98-86-2	C8H8O	120.15	745.93 , 1.313	4709771
81 benzoic acid, methyl ester	93-58-3	C8H8O2	136.15	765.928 , 1.267	212381
82 methyl salicylate	119-36-8	C8H8O3	152.15	833.922 , 1.254	680443
83 phenylmaleic anhydride	36122-35-7	C10H6O3	174.16	1013.9 , 1.472	1586579
84 phenol, 2-ethyl-4,5-dimethyl-	2219-78-5	C10H14O	150.22	773.928 , 1.096	456900
85 dibenzofuran	132-64-9	C12H8O	168.20	1013.9 , 1.406	72594
86 benzophenone	119-61-9	C13H10O	182.22	1061.9 , 1.459	991245
87 ethanedione, diphenyl-	134-81-6	C14H10O2	210.23	1141.89 , 1.538	220244
88 2-ethylhexyl salicylate	118-60-5	C15H22O3	250.34	1133.89 , 1.208	399828
89 homomenthyl salicylate	52253-93-7	C16H22O3	262.35	1169.89 , 1.261	847680

	monoterpenes				
90 thujene	58037-87-9	C10H16	136.24	629.942 , 1.023	804551
91 α -pinene	80-56-8	C10H16	136.24	637.941 , 1.036	10982041
92 <u>camphene</u>	79-92-5	C10H16	136.24	653.94 , 1.049	1465508
93 β -pinene	127-91-3	C10H16	136.24	673.938 , 1.036	195985
94 myrcene	123-35-3	C10H16	136.24	681.937 , 1.030	4059076
95 α -phellandrene	99-83-2	C10H16	136.24	697.935 , 1.043	740876
96 γ -terpinene	99-85-4	C10H16	136.24	705.934 , 1.043	330856
97 limonene	138-86-3	C10H16	136.24	717.933 , 1.063	51785894
98 ocimene	502-99-8	C10H16	136.24	725.932 , 1.030	247003
99 β -phellandrene	555-10-2	C10H16	136.24	737.931 , 1.049	962046
	oxygenated monoterpenes				
100 eucalyptol	470-82-6	C10H18O	154.25	721.933 , 1.076	88942381
101 linalool	78-70-6	C10H18O	154.25	761.929 , 1.063	790803
102 4-terpineol	562-74-3	C10H18O	154.25	821.923 , 1.122	464358
103 terpineol	98-55-5	C10H18O	154.25	829.922 , 1.168	2395168
	sesquiterpenes				
104 δ -cadinene	483-76-1	C15H24	204.36	1009.9 , 1.148	2617189
105 α -gurjunene	489-40-7	C15H24	204.36	1013.9 , 1.162	4411100
106 calamene	483-77-2	C15H22	204.36	1013.9 , 1.181	5298248
107 valencene	4630-07-3	C15H24	204.36	1021.9 , 1.175	981099
108 α -cubebene	17699-14-8	C15H24	204.36	921.913 , 1.063	1064541
109 copaene	3856-25-5	C15H24	204.36	937.911 , 1.096	13373209
110 aromadendrene isomer	n/a	C15H24	204.36	949.91 , 1.109	408678
111 isocaryophyllene	118-65-0	C15H24	204.36	957.909 , 1.109	2149275
112 caryophyllene	87-44-5	C15H24	204.36	965.908 , 1.129	25459553
113 <u>aromadendrene</u>	109119-91-7	C15H24	204.36	977.907 , 1.122	2335518
114 aromadendrene isomer	n/a	C15H24	204.36	981.907 , 1.142	3600670
115 humulene	6753-98-6	C15H24	204.36	985.906 , 1.142	5121282
116 α -selinene	473-13-2	C15H24	204.36	997.905 , 1.155	13362277

oxygenated sesquiterpenes						
117	palustrol	5986-49-2	C15H26O	222.37	1041.9 , 1.201	432673
S- or N-containing						
118	carbon disulfide	75-15-0	CS2	76.14	229.982 , 1.135	14363365
119	dimethyl sulfone	67-71-0	C2H6O2S	94.13	617.943 , 1.802	1370136
120	disulfide, dimethyl	624-92-0	C2H6S2	94.20	425.962 , 1.406	1053957
121	2-propenenitrile	107-13-1	C3H3N	53.06	221.983 , 1.327	452626
122	thiophene	110-02-1	C4H4S	81.14	329.972 , 1.551	1323859
123	1h-pyrrole-2,5-dione	541-59-3	C4H3NO2	97.02	677.937 , 1.485	497723
124	thiophene, 2-methyl-	554-14-3	C5H6S	98.17	457.959 , 1.313	304622
125	thiophene, 3-methyl-	616-44-4	C5H6S	98.17	469.958 , 1.300	318826
126	2-furancarbonitrile	617-90-3	C5H3NO	93.08	493.956 , 1.419	210175
127	thiophene, 2-ethyl-	872-55-9	C6H8S	112.19	569.948 , 1.188	566249
128	benzonitrile	100-47-0	C7H5N	103.12	681.937 , 1.353	1816982
129	benzothiazole	95-16-9	C7H5NS	135.19	853.92 , 1.445	245535
130	1h-isoindole-1,3(2h)-dione	85-41-6	C8H5NO2	147.13	977.907 , 1.571	203215
131	1,3,5-triazine-2,4-diamine, 6-phenyl-	91-76-9	C9H9N5	187.20	1221.88 , 1.841	795414
132	diethyltoluamide	134-62-3	C12H17NO	191.27	1033.9 , 1.340	5483653
Br-, Cl-, F-, or I-containing						
133	trichloromethane	67-66-3	CHCl3	119.38	273.978 , 1.366	563991
134	methylene chloride	75-09-2	CH2Cl2	84.93	225.982 , 1.201	173785426
135	methane, chloro-	74-87-3	CH3Cl	50.49	153.99 , 0.931	757061
136	methane, bromo-	74-83-9	CH3Br	94.40	197.985 , 0.983	30876744
137	methane, iodo-	74-88-4	CH3I	141.94	221.983 , 1.115	4908852
138	tetrachloroethylene	127-18-4	C2Cl4	165.83	505.954 , 1.168	818048
139	1,1-dichloro-1-fluoroethane	1717-00-6	C2H3Cl2F	116.95	209.984 , 1.010	47762552
140	benzene, 1,3,5-trifluoro-	372-38-3	C6H3F3	132.08	273.978 , 1.214	636582
141	benzene, 1,4-dichloro-	106-46-7	C6H4Cl2	147.00	705.934 , 1.181	1696894
142	benzene, chloro-	108-90-7	C6H5Cl	112.56	549.95 , 1.228	294823

142 total number of compounds meeting the peak selection criteria

15 compounds positively identified
127 compounds tentatively identified

Table S3. Positively identified compounds (**boldface**) and tentatively identified compounds in an SPME analysis using cleaned lab air ("CLA") passing over a sample of *Cedrus atlantica* (see GCxGC-TOFMS chromatogram in Figure 4). All peaks met the peak selection criteria.

	Name	CAS	Formula	MW	Isotope Ave. Retention Times (seconds)	Peak Area
alkanes, alkenes, alkynes, arenes						
1	benzene	71-43-2	C6H6	78.11	623.956 , 1.280	2620961
2	toluene	108-88-3	C7H8	92.14	799.938 , 1.228	345165
3	styrene	100-42-5	C8H8	104.15	979.92 , 1.320	543164
4	2-octene, (E)-	13389-42-9	C8H16	112.22	815.936 , 0.997	3218144
5	ethylbenzene	100-41-4	C8H10	115.24	935.924 , 1.195	256353
6	benzene, 1-ethyl-4-methyl-	622-96-8	C9H12	120.20	1063.91 , 1.175	183537
7	benzene, 1,3,5-trimethyl-	108-67-8	C9H12	120.20	1079.91 , 1.188	537559
8	benzene, 1,2,4-trimethyl-	95-63-6	C9H12	120.20	1111.91 , 1.228	195590
9	nonane	111-84-2	C9H20	128.26	963.922 , 0.970	451288
10	naphthalene	91-20-3	C10H8	128.17	1407.88 , 2.132	665757
11	benzene, 1,3-diethenyl-	108-57-6	C10H10	130.19	1267.89 , 1.663	265051
12	benzene, 1,2-diethenyl-	135-01-3	C10H10	130.19	1287.89 , 1.696	256481
13	benzene, 1-methyl-4-(1-methylethenyl)-	1195-32-0	C10H12	132.21	1219.9 , 1.432	1998790
14	benzene, 1-ethenyl-4-ethyl-	3454-07-7	C10H12	132.21	1235.89 , 1.452	504105
15	dehydrosabinene	36262-09-6	C10H14	134.22	1055.91 , 1.089	708834
16	p-cymene	99-87-6	C10H14	134.22	1135.9 , 1.201	2906253
17	2,6-octadiene, 2,6-dimethyl-	2792-39-4	C10H18	138.25	1159.9 , 1.353	824543
18	decane	124-18-5	C10H22	142.29	1083.91 , 0.977	116064
19	naphthalene, 1-methyl-	90-12-0	C11H10	142.20	1587.86 , 2.185	202717
20	undecane	1120-21-4	C11H24	156.31	1203.9 , 1.023	634001
21	dodecane	112-40-3	C12H26	170.34	1343.88 , 1.049	257671
22	tridecane	629-50-5	C13H28	184.37	1495.87 , 1.076	1935763
23	tetradecane	629-59-4	C14H30	198.39	1655.85 , 1.102	1026766
24	pentadecane	629-62-9	C15H32	212.42	1819.84 , 1.122	5571980
25	hexadecane	544-76-3	C16H34	226.45	1983.82 , 1.142	374365
26	heptadecane	629-78-7	C17H36	240.48	2147.8 , 1.162	1261832
27	octadecane	593-45-3	C18H38	254.50	2315.79 , 1.228	509686
28	nonadecane	629-92-5	C19H40	248.37	2523.77 , 1.327	798533

alcohols, ketones, aldehydes, furans

29	propanal	123-38-6	C3H6O	58.08	323.986 , 1.472	1308410
30	acetone	67-64-1	C3H6O	58.08	327.985 , 1.558	3266678
31	2(5h)-furanone	497-23-4	C4H4O2	84.07	995.918 , 3.432	181432
32	methacrolein	78-85-3	C4H6O	70.09	447.973 , 1.459	941476
33	2,3-dihydrofuran	1191-99-7	C4H6O	70.09	463.972 , 1.307	5396694
34	methyl vinyl ketone	78-94-4	C4H6O	70.09	483.97 , 1.604	262053
35	2-butenal, (E)-	123-73-9	C4H6O	70.09	599.958 , 1.624	4020719
36	butanedral	638-37-9	C4H6O2	86.09	791.939 , 2.739	2473750
37	butyrolactone	96-48-0	C4H6O2	86.09	995.918 , 2.587	7012279
38	ethene, ethoxy-	109-92-2	C4H8O	60.10	339.984 , 1.168	778948
39	butanal	123-72-8	C4H8O	72.11	487.969 , 1.346	1300707
40	2-butanone	78-93-3	C4H8O	72.11	495.968 , 1.399	525556
41	2-butene-1,4-diol	110-64-5	C4H8O2	88.11	995.918 , 2.112	848103
42	2,5-furandione, dihydro-3-methylene-	2170-03-8	C5H4O3	112.08	1023.92 , 2.713	351077
43	2-butenal, 3-methyl-	107-86-8	C5H8O	84.12	819.936 , 1.505	468644
44	pentanal	110-62-3	C5H10O	86.13	671.951 , 1.267	1048488
45	hexanal	66-25-1	C6H12O	100.16	831.935 , 1.228	2603733
46	2-pentanone, 3-methyl-	565-61-7	C6H12O	100.16	911.927 , 2.138	1208873
47	ethanol, 2-(2-ethoxyethoxy)-	111-90-0	C6H14O3	134.18	1087.91 , 1.808	8310745
48	3-methyl-3-cyclohexen-1-one	31883-98-4	C7H10O	110.16	1091.91 , 1.498	165813
49	2-heptenal, (Z)-	57266-86-1	C7H12O	112.17	1047.91 , 1.313	407535
50	heptanal	111-71-7	C7H14O	114.19	971.921 , 1.201	2003552
51	5-hexen-2-one, 5-methyl-3-methylene-	51756-18-4	C8H12O	124.18	951.923 , 1.148	561708
52	1-octen-3-one	4312-99-6	C8H14O	126.20	1067.91 , 1.228	439182
53	5-hepten-2-one, 6-methyl-	110-93-0	C8H14O	126.20	1075.91 , 1.261	810236
54	2-octenal, (E)-	2548-87-0	C8H14O	126.20	1171.9 , 1.426	844723
55	hexanal, 2-ethyl-	123-05-7	C8H16O	128.22	1043.91 , 1.135	645799
56	octanal	124-13-0	C8H16O	128.22	1095.91 , 1.201	6036517
57	1-hexanol, 2-ethyl-	104-76-7	C8H18O	130.23	1123.91 , 1.419	4249114
58	ethanone, 1-(4-methylphenyl)-	122-00-9	C9H10O	134.18	1383.88 , 2.231	8294137
59	nonanal	124-19-6	C9H18O	142.24	1223.9 , 1.327	15526808
60	2-butanol, 3-(2,2-dimethylpropoxy)-	74793-66-1	C9H20O2	160.26	2591.76 , 3.168	663854
61	decanal	112-31-2	C10H20O	156.27	1367.88 , 1.386	11892552

62	undecanal	112-44-7	C11H22O	170.30	1523.87 , 1.432	1605384
63	dodecanal	112-54-9	C12H24O	184.32	1687.85 , 1.472	790243
64	tetradecanal	124-25-4	C14H28O	212.38	1855.83 , 1.505	696317
65	pentadecanal	2765-11-9	C15H30O	226.40	2027.82 , 1.525	511270
66	hexadecanal	629-80-1	C16H32O	240.43	2191.8 , 1.564	1121389

ethers, carboxylic acids, esters

67	formic acid, propyl ester	110-74-7	C4H8O2	88.11	539.964 , 1.353	1777666
68	formic acid, butyl ester	592-84-7	C5H10O2	102.13	715.946 , 1.267	316125
69	2-propen-1-ol, 2-methyl-, acetate	820-71-3	C6H10O2	114.14	907.927 , 2.171	198696
70	hexanoic acid	142-62-1	C6H12O2	116.16	1031.91 , 3.326	696127
71	nonanoic acid	112-05-0	C9H18O2	150.18	1423.88 , 0.323	2478146
72	n-decanoic acid	334-48-5	C10H20O2	172.27	1579.86 , 0.277	2839978
73	dodecanoic acid	143-07-7	C12H24O2	200.32	1907.83 , 3.993	2979464

oxygenated aromatics

74	benzaldehyde	100-52-7	C7H6O	106.12	1067.91 , 1.749	2289358
75	acetophenone	98-86-2	C8H8O	120.15	1203.9 , 2.105	514994
76	cinnamaldehyde, (E)-	14371-10-9	C9H8O	132.16	1371.88 , 2.488	891974
77	2-propenal, 3-phenyl-	104-55-2	C9H8O	132.16	1399.88 , 2.581	754085
78	benzaldehyde, 4-ethyl-	4748-78-1	C9H10O	134.18	1343.88 , 2.053	1880544
79	benzaldehyde, 2,5-dimethyl-	5779-94-2	C9H10O	134.18	1371.88 , 2.132	1689715
80	benzoic acid, methyl ester	93-58-3	C8H8O2	136.15	1239.89 , 1.901	881170
81	ethanol, 2-phenoxy-	122-99-6	C8H10O2	138.17	1415.88 , 0.396	125712

monoterpene

82	<u>α-pinene</u>	80-56-8	C10H16	136.24	1027.92 , 1.030	49530814
83	<u>camphene</u>	79-92-5	C10H16	136.24	1051.91 , 1.056	2165139
84	<u>β-pinene</u>	127-91-3	C10H16	136.24	1083.91 , 1.069	70230291
85	<u>α-phellandrene</u>	99-83-2	C10H16	136.24	1111.91 , 1.102	356502
86	<u>limonene</u>	138-86-3	C10H16	136.24	1139.9 , 1.135	31451432
87	β-phellandrene	555-10-2	C10H16	136.24	1147.9 , 1.155	14067563
88	γ-terpinene	99-85-4	C10H16	136.24	1171.9 , 1.168	1036761
89	<u>terpinolene</u>	586-62-9	C10H16	136.24	1211.9 , 1.208	634624

oxygenated monoterpenes						
90	2(10)-pinen-3-one, (+/-)-	30460-92-5	C10H14O	150.22	1347.88 , 1.683	718335
91	myrtenal	564-94-3	C10H14O	150.22	1399.88 , 1.762	777887
92	l-trans-pinocarveol	547-61-5	C10H16O	152.24	1311.89 , 1.861	2011021
93	pinocamphone	547-60-4	C10H16O	152.24	1371.88 , 1.617	792416
94	<u>terpineol</u>	98-55-5	C10H18O	154.25	1371.88 , 1.828	357675
sesquiterpenes						
95	copaene	3856-25-5	C15H24	204.36	1683.85 , 1.261	2607970
96	β -bourbonene	5208-59-3	C15H24	204.36	1707.85 , 1.287	522222
97	<u>caryophyllene</u>	87-44-5	C15H24	204.36	1775.84 , 1.360	12160900
98	(Z,Z)- α -farnesene	n/a	C15H24	204.36	1779.84 , 1.366	598988
99	<u>humulene</u>	6753-98-6	C15H24	204.36	1835.83 , 1.426	2435809
100	α -muurolene	31983-22-9	C15H24	204.36	1879.83 , 1.426	1593179
oxygenated sesquiterpenes						
101	caryophyllene oxide	1139-30-6	C15H24O	220.36	2075.81 , 1.802	1665125
S- or N-containing						
102	benzonitrile	100-47-0	C7H5N	103.12	1095.91 , 1.967	1382417
<u>102</u>	<u>total number of compounds meeting the peak selection criteria</u>					
10	<u>compounds positively identified</u>					
92	<u>compounds tentatively identified</u>					

Table S4. Positively identified compounds (**boldface**) and tentatively identified compounds in an SPME analysis using uncleaned lab air ("ULA") passing over a sample of *Cedrus atlantica* (see GCxGC-TOFMS chromatogram in Figure 5). All peaks met the peak selection criteria.

	Name	CAS	Formula	Isotope Ave. Retention Times		Peak Area
				MW	(seconds)	
alkanes, alkenes, alkynes, arenes						
1	isoprene	78-79-5	C5H8	68.12	347.983 , 1.122	1996124
2	benzene	71-43-2	C6H6	78.11	623.956 , 1.294	5329035
3	cyclobutane, 1,2-bis(methylene)-	14296-80-1	C6H8	80.13	499.968 , 1.162	592448
4	isopropenylcyclopropane	4663-22-3	C6H10	82.15	519.966 , 1.089	493161
5	toluene	108-88-3	C7H8	92.14	799.938 , 1.234	3370916
6	styrene	100-42-5	C8H8	104.15	979.92 , 1.333	1492732
7	ethylbenzene	100-41-4 108-38-3;	C8H10	106.17	943.925, 1.200	2325646
8	<i>m</i> -xylene; <i>p</i> -xylene	106-42-3	C8H10	106.17	951.923 , 1.201	9966299
9	<i>o</i> -xylene	95-47-6	C8H10	106.17	983.92 , 1.234	1938829
10	2-octene, (E)-	13389-42-9	C8H16	112.22	815.936 , 0.997	3213783
11	octane	111-65-9	C8H18	114.23	827.935 , 0.983	650248
12	benzene, 1-propynyl-	673-32-5	C9H8	116.16	1183.9 , 1.637	211989
13	benzene, 2-propenyl-	300-57-2	C9H10	118.18	1107.91 , 1.333	1189718
14	indane	496-11-7	C9H10	118.18	1163.9 , 1.399	4236208
15	cumene	98-82-8	C9H12	120.20	1015.92 , 1.175	580175
16	benzene, propyl-	103-65-1	C9H12	120.20	1051.91 , 1.188	2546135
17	benzene, 1-ethyl-2-methyl-	611-14-3	C9H12	120.20	1059.91 , 1.188	13885282
18	benzene, 1-ethyl-4-methyl-	622-96-8	C9H12	120.20	1063.91 , 1.175	321359
19	benzene, 1,3,5-trimethyl-	108-67-8	C9H12	120.20	1075.91 , 1.201	64778489
20	benzene, 1,2,4-trimethyl-	95-63-6	C9H12	120.20	1107.91 , 1.241	18370218
21	benzene, 1,2,3-trimethyl-	526-73-8	C9H12	120.20	1147.9 , 1.327	10757123
22	nonane	111-84-2	C9H20	128.26	963.922 , 0.977	1285979
23	naphthalene	91-20-3	C10H8	128.17	1403.88 , 2.158	36867018
24	benzene, 1,3-diethenyl-	108-57-6	C10H10	130.19	1267.89 , 1.666	364275
25	benzene, 1,2-diethenyl-	135-01-3	C10H10	130.19	1287.89 , 1.698	256022
26	naphthalene, 1,2-dihydro-	447-53-0	C10H10	130.19	1335.88 , 1.736	1278177
27	benzene, 1-ethenyl-3-ethyl-	7525-62-4	C10H12	132.21	1219.9 , 1.431	3094592
28	benzene, 1-methyl-2-(1-methylethethyl)-	7399-49-7	C10H12	132.21	1223.9 , 1.439	16802786

29	benzene, 1-methyl-4-(2-propenyl)-	3333-13-9	C10H12	132.21	1239.89 , 1.472	3718549
30	1h-indene, 2,3-dihydro-5-methyl-	874-35-1	C10H12	148.21	1311.89 , 1.505	3176548
31	benzene, 1-methyl-2-(2-propenyl)-	1587-04-8	C10H12	132.21	1327.89 , 1.544	2326008
32	dehydrosabinene	36262-09-6	C10H14	134.22	1055.91 , 1.109	7441728
33	<i>2,6-dimethyl-1,3,5,7-octatetraene, E,E-</i>	460-01-5	C10H14	134.22	1091.91 , 1.148	26295077
34	<i>2,6-dimethyl-1,3,5,7-octatetraene, E,E-</i>	460-01-5	C10H14	134.22	1107.91 , 1.162	3355904
35	benzene, butyl-	104-51-8	C10H14	134.22	1115.91 , 1.188	554479
36	p-cymene	99-87-6	C10H14	134.22	1135.9 , 1.214	47077633
37	benzene, 1,3-diethyl-	141-93-5	C10H14	134.22	1163.9 , 1.247	1791560
38	benzene, 1-methyl-3-propyl-	1074-43-7	C10H14	134.22	1167.9 , 1.254	2464575
39	benzene, 1,4-diethyl-	105-05-5	C10H14	134.22	1175.9 , 1.261	8115050
40	benzene, 1-ethyl-2,4-dimethyl-	874-41-9	C10H14	134.22	1207.9 , 1.320	5593812
41	<i>2,6-dimethyl-1,3,5,7-octatetraene, E,E-</i>	460-01-5	C10H14	134.22	1251.89 , 1.360	4407461
42	benzene, 4-ethyl-1,2-dimethyl-	934-80-5	C10H14	134.22	1255.89 , 1.399	3250797
43	1,2,3,4,5,8-hexahydronaphthalene	36231-13-7	C10H14	134.22	1283.89 , 1.393	3915314
44	benzene, 2-ethyl-1,3-dimethyl-	2870-04-4	C10H14	134.22	1283.89 , 1.419	6069397
45	<i>2,6-dimethyl-1,3,5,7-octatetraene, E,E-</i>	460-01-5	C10H14	134.22	1291.89 , 1.406	2974025
46	bicyclo[3.2.1]oct-2-ene, 3-methyl-4-methylene-	49826-53-1	C10H14	134.22	1295.89 , 1.412	1775038
47	benzene, 1-methyl-2-(1-methylethyl)-	527-84-4	C10H14	134.22	1335.88 , 1.492	833709
48	3-octen-5-yne, 2,7-dimethyl-, (E)-	55956-33-7	C10H16	136.24	1027.92 , 1.063	227449713
49	2,4,6-trimethyl-1,3,6-heptatriene	24648-33-7	C10H16	136.24	1579.86 , 1.577	2413552
50	cyclohexene, 3-methyl-6-(1-methylethyl)-	5256-65-5	C10H18	138.25	1131.9 , 1.089	348823
51	2,6-octadiene, 2,6-dimethyl-	2792-39-4	C10H18	138.25	1159.9 , 1.366	2936375
52	nonane, 2-methyl-	871-83-0	C10H22	142.29	1043.91 , 0.977	2889555
53	decane	124-18-5	C10H22	142.29	1083.91 , 1.003	990912
54	naphthalene, 2-methyl-	91-57-6	C11H10	142.20	1587.86 , 2.204	4304109
55	naphthalene, 1-methyl-	90-12-0	C11H10	142.20	1615.86 , 2.290	1480403
56	1h-indene, 1,1-dimethyl-	18636-55-0	C11H12	144.22	1499.87 , 1.782	806976
57	1h-indene, 2,3-dihydro-1,6-dimethyl-	17059-48-2	C11H14	146.23	1371.88 , 1.459	209969
58	1h-indene, 2,3-dihydro-1,1-dimethyl-	4912-92-9	C11H14	146.23	1375.88 , 1.478	331220
59	1h-indene, 2,3-dihydro-1,3-dimethyl-	4175-53-5	C11H14	146.23	1395.88 , 1.518	935472
60	benzene, 1-methyl-3-(1-methyl-2-propenyl)-	52161-57-6	C11H14	146.23	1415.88 , 1.551	2190165
61	1h-indene, 2,3-dihydro-4,7-dimethyl-	6682-71-9	C11H14	146.23	1483.87 , 1.604	278965
62	naphthalene, 1,2,3,4-tetrahydro-5-methyl-	2809-64-5	C11H14	146.23	1507.87 , 1.650	981635
63	benzene, 1-methyl-4-(1-methylpropyl)-	1595-16-0	C11H16	148.25	1291.89 , 1.327	387523

64	benzene, 1,3-diethyl-5-methyl-	2050-24-0	C11H16	148.25	1331.88 , 1.366	210432
65	benzene, 1,3-dimethyl-5-(1-methylethyl)-	4706-90-5	C11H16	148.25	1387.88 , 1.439	406272
66	benzene, 1-ethyl-4-(1-methylethyl)-	4218-48-8	C11H16	148.25	1403.88 , 1.459	261063
67	7-methyl-1,2,3,5,8,8a-hexahydronaphthalene	107914-88-5	C11H16	148.25	1483.87 , 1.492	715560
68	naphthalene, decahydro-2-methyl-	2958-76-1	C11H20	152.28	1271.89 , 1.155	630080
69	1-methyldecahydronaphthalene	2958-75-0	C11H20	152.28	1295.89 , 1.181	546429
70	cyclohexane, pentyl-	4292-92-6	C11H22	154.30	1275.89 , 1.102	1528522
71	1-decene, 8-methyl-	61142-79-8	C11H22	154.30	1567.86 , 1.815	2755453
72	decane, 4-methyl-	2847-72-5	C11H24	156.31	1111.91 , 0.990	1553797
73	decane, 3-methyl-	13151-34-3	C11H24	156.31	1167.9 , 1.016	2717472
74	undecane	1120-21-4	C11H24	156.31	1203.9 , 1.030	21282734
75	decane, 2-methyl-	6975-98-0	C11H24	156.31	1243.89 , 1.030	5531477
76	biphenyl	92-52-4	C12H10	154.21	1699.85 , 2.422	619759
77	naphthalene, 2-ethyl-	939-27-5	C12H12	156.23	1743.84 , 2.211	160942
78	naphthalene, 2,3-dimethyl-	581-40-8	C12H12	156.23	1775.84 , 2.211	766682
79	naphthalene, 1,4-dimethyl-	571-58-4	C12H12	156.23	1799.84 , 2.303	679866
80	naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	4175-54-6	C12H16	160.26	1595.86 , 1.624	983227
81	naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	1985-59-7	C12H16	160.26	1883.83 , 3.056	733312
82	benzene, (1,3-dimethylbutyl)-	19219-84-2	C12H18	162.28	1483.87 , 1.419	205782
83	benzene, (2,2-dimethylbutyl)-	28080-86-6	C12H18	162.28	1627.86 , 2.178	2982441
84	1-dodecene	112-41-4	C12H24	168.32	1331.88 , 1.096	2081931
85	cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	C12H24	168.32	1359.88 , 1.109	671892
86	cyclohexane, hexyl-	4292-75-5	C12H24	168.32	1427.88 , 1.142	944012
87	undecane, 3-methyl-	1002-43-3	C12H26	170.34	1263.89 , 1.036	5230310
88	undecane, 2-methyl-	7045-71-8	C12H26	170.34	1291.89 , 1.043	20865674
89	undecane, 3-methyl-	1002-43-3	C12H26	170.34	1303.89 , 1.049	3764279
90	dodecane	112-40-3	C12H26	170.34	1339.88 , 1.063	16281476
91	diphenylmethane	101-81-5	C13H12	168.24	1875.83 , 2.402	284019
92	decane, 2,6,7-trimethyl-	62108-25-2	C13H28	184.37	1363.88 , 1.049	3928258
93	undecane, 5-ethyl-	17453-94-0	C13H28	184.37	1403.88 , 1.063	1159762
94	decane, 2,3,4-trimethyl-	62238-15-7	C13H28	184.37	1431.87 , 1.069	3262111
95	dodecane, 3-methyl-	17312-57-1	C13H28	184.37	1451.87 , 1.076	1349428
96	tridecane	629-50-5	C13H28	184.37	1491.87 , 1.089	3939090
97	3-tetradecene, (Z)-	41446-67-7	C14H28	196.38	1639.85 , 1.155	2601645
98	tridecane, 3-methyl-	6418-41-3	C14H30	198.39	1607.86 , 1.102	476444

99	tetradecane	629-59-4	C14H30	198.39	1651.85 , 1.115	4370142
100	α -calacorene	21391-99-1	C15H20	200.33	1967.82 , 1.723	400587
101	1,8-cyclopentadecadiyne	4722-42-3	C15H22	202.34	1815.84 , 1.492	3844181
102	naphthalene, 1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methyleth-	483-77-2	C15H22	202.34	1923.83 , 1.597	585583
103	1,6,10-dodecatriene, 7,11-dimethyl-3-methylene-, (E)-	18794-84-8	C15H24	204.36	1755.84 , 1.340	29607805
104	pentadecane	629-62-9	C15H32	212.42	1815.84 , 1.135	18236143
105	hexadecane	544-76-3	C16H34	226.45	1983.82 , 1.155	2975795
106	heptadecane	629-78-7	C17H36	240.48	2143.8 , 1.175	7696416
107	heptadecane, 2-methyl-	1560-89-0	C18H38	254.50	2251.79 , 1.201	634774
108	octadecane	593-45-3	C18H38	254.50	2315.79 , 1.241	9691037
109	1-nonadecene	18435-45-5	C19H38	266.51	2303.79 , 1.294	1817592
110	heptadecane, 2,6-dimethyl-	54105-67-8	C19H40	268.53	2163.8 , 1.135	1561644
111	octadecane, 2-methyl-	1560-88-9	C19H40	268.53	2443.77 , 1.280	886843
112	nonadecane	629-92-5	C19H40	268.53	2519.77 , 1.333	12829843
113	hexadecane, 2,6,10,14-tetramethyl-	638-36-8	C20H42	282.56	2343.78 , 1.208	1796934

alcohols, ketones, aldehydes, furans

114	propanal	123-38-6	C3H6O	58.08	323.986 , 1.485	550451
115	acetone	67-64-1	C3H6O	58.08	327.985 , 1.571	21737864
116	2(5h)-furanone	497-23-4	C4H4O2	84.07	995.918 , 3.43	172432
117	methacrolein	78-85-3	C4H6O	70.09	447.973 , 1.465	6091629
118	2,3-dihydrofuran	1191-99-7	C4H6O	70.09	463.972 , 1.320	8343425
119	methyl vinyl ketone	78-94-4	C4H6O	70.09	483.97 , 1.617	1417475
120	2-butenal, (E)-	123-73-9	C4H6O	70.09	599.958 , 1.643	2684848
121	butyrolactone	96-48-0	C4H6O2	86.09	995.918 , 2.614	13598792
122	ethene, ethoxy-	109-92-2	C4H8O	60.10	339.984 , 1.168	793774
123	butanal	123-72-8	C4H8O	72.11	483.97 , 1.373	2106421
124	2-butanone	78-93-3	C4H8O	72.11	495.968 , 1.412	1677699
125	2-butene-1,4-diol	110-64-5	C4H8O2	88.11	995.918 , 2.138	176092
126	2,5-furandione, dihydro-3-methylene-	2170-03-8	C5H4O3	112.08	1023.92 , 2.746	524365
127	2-pentanone	107-87-9	C5H10O	86.13	655.952 , 1.307	626169
128	cyclopentanol	96-41-3	C5H10O	86.13	671.951 , 1.287	2293899
129	furan, 3-methyl-	930-27-8	C5H6O	82.10	527.965 , 1.320	12908838
130	2-butenal, 3-methyl-	107-86-8	C5H8O	84.12	819.936 , 1.518	1133940
131	3-penten-2-one, 4-methyl-	141-79-7	C6H10O	98.15	839.934 , 1.320	694989

132	2(3h)-furanone, 5-ethyldihydro-	695-06-7	C6H10O2	114.14	1175.9 , 2.369	473823
133	methyl isobutyl ketone	108-10-1	C6H12O	100.16	747.943 , 1.228	675007
134	3-pentanone, 2-methyl-	565-69-5	C6H12O	100.16	759.942 , 1.201	1230086
135	hexanal	66-25-1	C6H12O	100.16	831.935 , 1.241	4046031
136	3-hexen-1-ol, (Z)-	928-96-1	C6H12O	100.16	903.928 , 1.696	1226902
137	2-pentanone, 3-methyl-	565-61-7	C6H12O	100.16	911.927 , 2.136	371293
138	1-hexanol	111-27-3	C6H14O	102.18	915.926 , 1.544	3752411
139	ethanol, 2-(2-ethoxyethoxy)-	111-90-0	C6H14O3	134.18	1083.91 , 1.828	13774460
140	3-methyl-3-cyclohexen-1-one	31883-98-4	C7H10O	110.16	1091.91 , 1.511	1690248
141	2-heptenal, (Z)-	57266-86-1	C7H12O	112.17	1047.91 , 1.327	3330610
142	3-heptanone	106-35-4	C7H14O	114.19	951.923 , 1.195	5091808
143	2-heptanone	110-43-0	C7H14O	114.19	959.922 , 1.221	8142756
144	heptanal	111-71-7	C7H14O	114.19	971.921 , 1.214	2470036
145	2-heptanol	543-49-7	C7H16O	116.20	959.922 , 1.353	8874599
146	1-heptanol	111-70-6	C7H16O	116.20	1043.91 , 1.459	2721717
147	oxepine, 2,7-dimethyl-	1487-99-6	C8H10O	122.17	1019.92 , 1.228	479956
148	1-octen-3-one	4312-99-6	C8H14O	126.20	1067.91 , 1.241	1304136
149	5-hepten-2-one, 6-methyl-	110-93-0	C8H14O	126.20	1075.91 , 1.280	3435691
150	2-octenal, (E)-	2548-87-0	C8H14O	126.20	1171.9 , 1.445	2747406
151	2(3h)-furanone, 5-butyldihydro-	104-50-7	C8H14O2	142.20	1475.87 , 2.660	105152
152	2-heptanone, 6-methyl-	928-68-7	C8H16O	128.22	1039.91 , 1.201	1619159
153	hexanal, 2-ethyl-	123-05-7	C8H16O	128.22	1043.91 , 1.135	242419
154	3-heptanone, 5-methyl-	541-85-5	C8H16O	128.22	1071.91 , 1.188	75288632
155	2-octanone	111-13-7	C8H16O	128.22	1079.91 , 1.214	3803964
156	octanal	124-13-0	C8H16O	128.22	1095.91 , 1.214	30056978
157	1-hexanol, 2-ethyl-	104-76-7	C8H18O	130.23	1115.91 , 1.432	3781521
158	1-octanol	111-87-5	C8H18O	130.23	1163.9 , 1.584	374551399
159	ethanone, 1-(4-methylphenyl)-	122-00-9	C9H10O	134.18	1379.88 , 2.264	54578814
160	4-acetyl-1-methylcyclohexene	6090-09-1	C9H14O	138.21	1283.89 , 1.676	1747890
161	2-nonanone	821-55-6	C9H18O	142.24	1203.9 , 1.340	33669000
162	nonanal	124-19-6	C9H18O	142.24	1219.9 , 1.340	48085519
163	2-nonal	628-99-9	C9H20O	144.26	1203.9 , 1.478	8865528
164	1-nonal	143-08-8	C9H20O	144.26	1299.89 , 1.723	23594412
165	1,7-octadien-3-one, 2-methyl-6-methylene-	41702-60-7	C10H14O	150.22	1275.89 , 1.571	25307754
166	2,6-octadienal, 3,7-dimethyl-, (E)-	141-27-5	C10H16O	152.24	1175.9 , 1.082	1103220

167	1,5,7-octatrien-3-ol, 2,6-dimethyl-	29414-56-0	C10H16O	152.24	1287.89 , 2.033	13168600
168	2,6-octadienal, 3,7-dimethyl-	5392-40-5	C10H16O	152.24	1343.88 , 1.861	14998024
169	decanal	112-31-2	C10H20O	156.27	1363.88 , 1.399	27674872
170	2-undecanone	112-12-9	C11H22O	170.30	1499.87 , 1.452	6025413
171	undecanal	112-44-7	C11H22O	170.30	1519.87 , 1.459	26239031
172	1-undecanol	112-42-5	C11H24O	172.31	1611.86 , 1.828	3092109
173	dodecanal	112-54-9	C12H24O	184.32	1687.85 , 1.492	5761544
174	5,9-undecadien-2-one, 6,10-dimethyl-, (E)-	3796-70-1	C13H22O	194.32	1759.84 , 1.696	1531848
175	tetradecanal	124-25-4	C14H28O	212.38	1855.83 , 1.505	765725
176	pentadecanal	2765-11-9	C15H30O	226.40	2027.82 , 1.525	1211760
177	hexadecanal	629-80-1	C16H32O	240.43	2191.8 , 1.564	2665073

ethers, carboxylic acids, esters

178	formic acid, propyl ester	110-74-7	C4H8O2	88.11	539.964 , 1.353	1348879
179	formic acid, butyl ester	592-84-7	C5H10O2	102.13	715.946 , 1.262	277575
180	2-butenoic acid, 3-methyl-, methyl ester	924-50-5	C6H10O2	114.14	903.928 , 1.274	1730298
181	2-propen-1-ol, 2-methyl-, acetate	820-71-3	C6H10O2	114.14	907.927 , 2.169	87833
182	2-butenoic acid, 2-methyl-, methyl ester	41725-90-0	C6H10O2	114.14	927.925 , 1.274	8822307
183	butanoic acid, 3-methyl-, methyl ester	556-24-1	C6H12O2	116.16	795.938 , 1.175	2988552
184	acetic acid, butyl ester	123-86-4	C6H12O2	116.16	847.933 , 1.188	1780655
185	hexanoic acid	142-62-1	C6H12O2	116.16	1031.91 , 3.406	471232
186	ethanol, 2-butoxy-	111-76-2	C6H14O2	118.18	971.921 , 1.577	525819
187	2-buten-1-ol, 3-methyl-, acetate	1191-16-8	C7H12O2	128.17	987.919 , 1.254	3052318
188	2-pentenoic acid, 3-methyl-, methyl ester	50652-79-4	C7H12O2	128.17	1035.91 , 1.247	884964
189	2-pentanol, acetate	626-38-0	C7H14O2	130.19	895.928 , 1.142	622644
190	1-butanol, 3-methyl-, acetate	123-92-2	C7H14O2	130.19	935.924 , 1.155	3459729
191	hexanoic acid, 4-methylene-, methyl ester	73805-48-8	C8H14O2	142.20	1115.91 , 1.267	506985
192	acetic acid, hexyl ester	142-92-7	C8H16O2	144.21	1095.91 , 1.168	26432384
193	2-butoxyethyl acetate	112-07-2	C8H16O3	160.21	1179.9 , 1.406	2722927
194	nonanoic acid	112-05-0	C9H18O2	150.18	1423.88 , 4.320	731800
195	2-propenoic acid, 3-phenyl-, methyl ester	103-26-4	C10H10O2	162.19	1687.85 , 2.759	426475
196	acetic acid, octyl ester	112-14-1	C10H20O2	172.27	1355.88 , 1.333	55253157
197	n-decanoic acid	334-48-5	C10H20O2	172.27	1579.86 , 4.256	826523
198	2,6-octadienoic acid, 3,7-dimethyl-, methyl ester	2349-14-6	C11H18O2	182.26	1543.86 , 1.604	12309908
199	2-decanoic acid, methyl ester, (E)-	7367-85-3	C11H20O2	184.28	1531.86 , 1.472	6746666

200	acetic acid, nonyl ester	143-13-5	C11H22O2	186.30	1507.87 , 1.379	938650
201	acetic acid, 1,7,7-trimethyl-bicyclo[2.2.1]hept-2-yl ester	92618-89-8	C12H20O2	196.29	1519.87 , 1.478	31853578
202	2,6-octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-	141-12-8	C12H20O2	196.29	1595.86 , 1.571	3411851
203	dodecanoic acid	143-07-7	C12H24O2	200.32	1907.83 , 4.112	1610974
204	propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-meth-	74367-33-2	C12H24O3	216.32	1635.85 , 2.000	83682383
205	propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl e	74367-34-3	C12H24O3	216.32	1655.85 , 1.855	85383205
206	z-11-tetradecenoic acid	79039-46-6	C14H26O2	226.36	2307.79 , 2.132	11952176
207	propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,;	74381-40-1	C16H30O4	286.41	2019.82 , 1.472	11268952
208	n-hexadecanoic acid	57-10-3	C16H32O2	256.43	2663.75 , 2.330	2919808

oxygenated aromatics

209	benzaldehyde	100-52-7	C7H6O	106.12	1067.91 , 1.762	4641707
210	oxepine, 2,7-dimethyl-	1487-99-6	C8H10O	122.17	1019.92 , 1.228	479956
211	phenylethyl alcohol	60-12-8	C8H10O	122.17	1251.89 , 3.267	1018401
212	ethanol, 2-phenoxy-	122-99-6	C8H10O2	138.17	1415.88 , 4.296	120012
213	benzeneacetaldehyde	122-78-1	C8H8O	120.15	1159.9 , 2.053	124890
214	acetophenone	98-86-2	C8H8O	120.15	1203.9 , 2.119	1831416
215	benzaldehyde, 3-methyl-	620-23-5	C8H8O	120.15	1207.9 , 2.026	433646
216	benzoic acid, methyl ester	93-58-3	C8H8O2	136.15	1239.89 , 1.907	1175181
217	methyl salicylate	119-36-8	C8H8O3	152.15	1395.88 , 2.237	688663
218	cinnamaldehyde, (E)-	14371-10-9	C9H8O	132.16	1371.88 , 2.508	1283500
219	2-propenal, 3-phenyl-	104-55-2	C9H8O	132.16	1399.88 , 2.614	1225245
220	benzeneacetaldehyde, α -methyl-	93-53-8	C9H10O	134.18	1119.91 , 1.195	282066
221	benzaldehyde, 4-ethyl-	4748-78-1	C9H10O	134.18	1339.88 , 2.079	2209910
222	benzaldehyde, 2,5-dimethyl-	5779-94-2	C9H10O	134.18	1367.88 , 2.158	2453104
223	acetic acid, phenylmethyl ester	140-11-4	C9H10O2	152.19	1315.89 , 2.092	860146
224	benzoic acid, 3-methyl-, methyl ester	99-36-5	C9H10O2	150.18	1399.88 , 2.020	2588158
225	benzoic acid, 4-methyl-, methyl ester	99-75-2	C9H10O2	150.18	1415.88 , 2.053	296839
226	benzenemethanol, α,α -dimethyl-	617-94-7	C9H12O	136.19	1211.9 , 2.376	1354293
227	phenol, 2,4,6-trimethyl-	527-60-6	C9H12O	136.19	1387.88 , 3.241	1324601
228	benzenopropanol	122-97-4	C9H12O	136.19	1419.88 , 3.472	1521192
229	benzoic acid, 4-acetyl-, methyl ester	3609-53-8	C10H10O3	178.19	1851.83 , 3.524	512867
230	propiophenone, 2'-methyl-	2040-14-4	C10H12O	148.21	1527.87 , 2.204	285518
231	acetic acid, 2-phenylethyl ester	103-45-7	C10H12O2	164.20	1455.87 , 2.138	11302034
232	benzenemethanol, $\alpha,\alpha,4$ -trimethyl-	1197-01-9	C10H14O	150.22	1355.88 , 2.422	11631294

233	3-penten-2-one, 5-phenyl-	10521-97-8	C11H12O	160.22	1591.86 , 2.409	1866718
234	benzene, 2-methoxy-4-methyl-1-(1-methylethyl)-	1076-56-8	C11H16O	164.25	1411.88 , 1.531	4669382
235	diethyl phthalate	84-66-2	C12H14O4	222.24	2019.82 , 3.062	1376819
236	benzophenone	119-61-9	C13H10O	182.22	2123.81 , 3.551	249911
237	1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	C16H22O4	278.35	2511.77 , 3.333	504636

monoterpenes

238	thujene	58037-87-9	C10H16	136.24	1011.92 , 1.043	7665208
239	<u>α-pinene</u>	80-56-8	C10H16	136.24	1031.91 , 1.016	45854233
240	<u>camphene</u>	79-92-5	C10H16	136.24	1051.91 , 1.082	83318541
241	sabinene	3387-41-5	C10H16	136.24	1071.91 , 1.082	31949966
242	<u>myrcene</u>	123-35-3	C10H16	136.24	1075.91 , 1.148	107325890
243	<u>β-pinene</u>	127-91-3	C10H16	136.24	1083.91 , 1.069	849487924
244	<u>α-phellandrene</u>	99-83-2	C10H16	136.24	1107.91 , 1.115	24909760
245	<u>δ³-carene</u>	13466-78-9	C10H16	136.24	1111.91 , 1.122	8537684
246	cyclohexene, 4-methyl-3-(1-methylethylidene)-	99805-90-0	C10H16	136.24	1119.91 , 1.122	932428
247	<u>γ-terpinene</u>	99-85-4	C10H16	136.24	1123.91 , 1.129	16867395
248	<u>limonene</u>	138-86-3	C10H16	136.24	1139.9 , 1.148	832182499
249	<u>β-phellandrene</u>	555-10-2	C10H16	136.24	1143.9 , 1.168	225258364
250	<u>γ-terpinene</u>	99-85-4	C10H16	136.24	1167.9 , 1.181	26722232
251	<u>terpinolene</u>	586-62-9	C10H16	136.24	1211.9 , 1.228	99984355

oxygenated monoterpenes

252	bicyclo[3.3.0]oct-2-en-7-one, 6-methyl-	n/a	C9H12O	136.19	1351.88 , 2.039	704198
253	<u>(1r)-(+)-nopinone</u>	38651-65-9	C9H14O	138.21	1315.89 , 1.789	2557432
254	cryptone	500-02-7	C9H14O	138.21	1387.88 , 1.934	1316357
255	2(10)-pinen-3-one, (+/-)-	30460-92-5	C10H14O	150.22	1347.88 , 1.696	20451022
256	myrtenal	564-94-3	C10H14O	150.22	1395.88 , 1.789	17899333
257	1-verbenone	1196-01-6	C10H14O	150.22	1431.87 , 1.980	7807307
258	carvone	99-49-0	C10H14O	150.22	1459.87 , 1.954	3899902
259	<u>α-thujenal</u>	57129-54-1	C10H14O	150.22	1495.87 , 2.026	391363
260	<u>d-verbenol</u>	473-67-6	C10H16O	152.24	1207.9 , 1.723	20529245
261	<u>d-verbenol</u>	473-67-6	C10H16O	152.24	1223.9 , 1.597	1270037
262	<u>α-pinene epoxide</u>	1686-14-2	C10H16O	152.24	1255.89 , 1.386	2038528
263	2-cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, trans-	7212-40-0	C10H16O	152.24	1263.89 , 1.789	6251762

264	2-cyclohexen-1-ol, 1-methyl-4-(1-methylethenyl)-, <i>trans</i> -	7212-40-0	C10H16O	152.24	1283.89 , 1.888	1641024
265	limonene oxide, <i>cis</i> -	4680-24-4	C10H16O	152.24	1287.89 , 1.439	7751350
266	<i>cis</i> -verbenol	18881-04-4	C10H16O	152.24	1299.89 , 1.841	2513720
267	<i>d</i> -verbenol	473-67-6	C10H16O	152.24	1307.89 , 1.901	74929781
268	<i>l</i> - <i>trans</i> -pinocarveol	547-61-5	C10H16O	152.24	1311.89 , 1.861	1830892
269	bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-	18358-53-7	C10H16O	152.24	1347.88 , 1.577	4359620
270	cyclohexanol, 2-methylene-5-(1-methylethenyl)-	35907-10-9	C10H16O	152.24	1359.88 , 2.204	2550296
271	pinocamphone	547-60-4	C10H16O	152.24	1367.88 , 1.637	25026469
272	myrtenol	515-00-4	C10H16O	152.24	1379.88 , 2.178	9121331
273	myrtanal	4764-14-1	C10H16O	152.24	1391.88 , 1.657	1151390
274	<i>cis</i> -carveol	1197-06-4	C10H16O	152.24	1403.88 , 2.244	2637729
275	3-carvomenthenone	89-81-6	C10H16O	152.24	1487.87 , 1.927	370123
276	bicyclo[3.1.0]hex-3-en-2-ol, 2-methyl-5-(1-methylethyl)-, (1 α 97631-68-0	97631-68-0	C10H16O	152.24	1515.87 , 1.544	2465591
277	<u>linalool</u>	78-70-6	C10H18O	154.25	1211.9 , 1.544	3198948
278	menthone	10458-14-7	C10H18O	154.25	1327.89 , 1.459	798060
279	borneol	464-45-9	C10H18O	154.25	1343.88 , 1.954	1617443
280	<u>4-terpinenol</u>	562-74-3	C10H18O	154.25	1351.88 , 1.650	12147293
281	<u>terpineol</u>	98-55-5	C10H18O	154.25	1371.88 , 1.835	24682347
282	menthol	1490-04-6	C10H20O	156.27	1343.88 , 1.709	1684116
283	trans-pinocaryl acetate	1686-15-3	C12H18O2	194.27	1535.86 , 1.577	4671118
284	myrtenyl acetate	1079-01-2	C12H18O2	194.27	1571.86 , 1.617	7163020
285	fenchyl acetate	13851-11-1	C12H20O2	196.29	1415.88 , 1.366	1293329

sesquiterpenes

286	α -cubebene	17699-14-8	C15H24	204.36	1623.86 , 1.241	4471021
287	α -longipinene	5989-08-2	C15H24	204.36	1659.85 , 1.280	32757290
288	copaene	3856-25-5	C15H24	204.36	1679.85 , 1.254	233067207
289	β -cubebene	13744-15-5	C15H24	204.36	1695.85 , 1.307	3815704
290	cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-	110823-68-2	C15H24	204.36	1699.85 , 1.360	1569263
291	β -bourbonene	5208-59-3	C15H24	204.36	1703.85 , 1.300	7013300
292	longicyclene	1137-12-8	C15H24	204.36	1707.85 , 1.307	2488949
293	δ -elemene	20307-84-0	C15H24	204.36	1735.84 , 1.320	2593004
294	isocaryophyllene	118-65-0	C15H24	204.36	1739.84 , 1.360	3998439
295	β -patchoulene	514-51-2	C15H24	204.36	1743.84 , 1.373	10336617
296	<i>cis</i> - α -bisabolene	29837-07-8	C15H24	204.36	1751.84 , 1.353	3528444

297	<i>aromadendrene isomer</i>	n/a	C15H24	204.36	1759.84 , 1.366	1826753
298	longifolene	475-20-7	C15H24	204.36	1763.84 , 1.379	57414380
299	<u>α-cedrene</u>	469-61-4	C15H24	204.36	1767.84 , 1.388	215432121
300	<u>caryophyllene</u>	87-44-5	C15H24	204.36	1771.84 , 1.406	250034001
301	(Z,Z)- α -farnesene	n/a	C15H24	204.36	1779.84 , 1.367	115386
302	<u>aromadendrene</u>	489-39-4	C15H24	204.36	1803.84 , 1.386	3555813
303	<u>humulene</u>	6753-98-6	C15H24	204.36	1831.83 , 1.412	202867501
304	α -farnesene	502-61-4	C15H24	204.36	1839.83 , 1.399	9373769
305	<i>germacrene d</i>	23986-74-5	C15H24	204.36	1847.83 , 1.300	4191409
306	α -muurolene	31983-22-9	C15H24	204.36	1847.83 , 1.426	2545102
307	β -cubebene	13744-15-5	C15H24	204.36	1855.83 , 1.307	611456
308	(Z)- α -farnesene	28973-97-9	C15H24	204.36	1855.83 , 1.445	9677194
309	α -amorphene	483-75-0	C15H24	204.36	1875.83 , 1.439	51198588
310	(Z,E)- α -farnesene	26560-14-5	C15H24	204.36	1879.83 , 1.426	9968377
311	calarene	17334-55-3	C15H24	204.36	1887.83 , 1.478	4505739
312	clove	469-92-1	C15H24	204.36	1891.83 , 1.478	1396279
313	δ -cadinene	483-76-1	C15H24	204.36	1907.83 , 1.459	5520646
314	<i>germacrene d</i>	23986-74-5	C15H24	204.36	1911.83 , 1.485	2389564
315	naphthalene, 1,2,3,4,4 α ,7-hexahydro-1,6-dimethyl-4-(1-methyl-	16728-99-7	C15H24	204.36	1939.82 , 1.505	819736

oxygenated sesquiterpenes

316	<i>longipinocarvone</i>	65556-52-7	C15H22O	218.34	2043.81 , 1.980	18302311
317	<i>caryophyllene oxide</i>	1139-30-6	C15H24O	220.36	2063.81 , 1.802	1780903
318	germacrone	6902-91-6	C15H22O	218.34	2071.81 , 1.987	5311563
319	<i>caryophyllene oxide</i>	1139-30-6	C15H24O	220.36	2071.81 , 1.828	47177954
320	<i>longipinocarvone</i>	65556-52-7	C15H22O	218.34	2079.81 , 2.006	2599088
321	<i>caryophyllene oxide</i>	1139-30-6	C15H24O	220.36	2091.81 , 1.848	1167628
322	humulene epoxide 2	19888-34-7	C15H24O	220.36	2115.81 , 1.894	9186641
323	tetracyclo[6.3.2.0(2,5).0(1,8)]tridecan-9-ol, 4,4-dimethyl-	n/a	C15H24O	220.36	2135.8 , 2.462	18055427
324	<i>caryophyllene oxide</i>	1139-30-6	C15H24O	220.36	2183.8 , 2.614	2714078
325	trans-Z- α -bisabolene epoxide	111536-37-9	C15H24O	220.36	2187.8 , 2.620	3126672

S-, or N-containing

326	dimethyl sulfide	75-18-3	C2H6S	62.13	363.982 , 1.274	429556
327	benzonitrile	100-47-0	C7H5N	103.12	1091.91 , 1.987	1857225

328	benzothiazole	95-16-9	C7H5NS	135.19	1455.87 , 3.023	2056556
329	benzene, 2,4-diisocyanato-1-methyl-	584-84-9	C9H6N2O2	174.16	1639.85 , 2.152	21414874

Br-, Cl-, F-, or I-containing

330	benzene, 1,3-dichloro-	541-73-1	C6H4Cl2	147.00	1131.9 , 1.511	805536
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330 total number of compounds meeting the peak selection criteria

18 compounds positively identified

312 compounds tentatively identified

Table S5. Positively identified compounds (**boldface**) and tentatively identified compounds in an ATD analysis using cleaned lab air ("CLA") passing over a sample of *Cedrus atlantica* (see GCxGC-TOFMS chromatogram in Figure 6). All peaks met the peak selection criteria.

Name	CAS	Formula	Isotope Ave.	Retention Time (seconds)	Peak Area
alkanes, alkenes, alkynes, arenes					
1 1,3-cyclopentadiene	542-92-7	C5H6	66.10	423.976 , 1.168	588021
2 <u>isoprene</u>	78-79-5	C5H8	68.12	375.98 , 1.089	15353663
3 1-butene, 3-methyl-	563-45-1	C5H10	70.14	371.981 , 1.036	297906
4 2-pentene	109-68-2	C5H10	70.14	387.979 , 1.043	403891
5 cyclopropane, ethyl-	1191-96-4	C5H10	70.14	459.972 , 1.023	3117905
6 butane, 2-methyl-	78-78-4	C5H12	72.15	331.985 , 0.805	316439
7 pentane	109-66-0	C5H12	72.15	359.982 , 1.003	10036602
8 cyclopentane, methyl-	96-37-7	C6H12	84.16	563.962 , 1.016	2281292
9 cyclohexane	110-82-7	C6H12	84.16	623.956 , 1.023	952811
10 pentane, 2-methyl-	107-83-5	C6H14	86.18	459.972 , 1.003	1846476
11 pentane, 3-methyl-	96-14-0	C6H14	86.18	483.97 , 1.003	1631502
12 hexane	110-54-3	C6H14	86.18	511.967 , 1.003	4022034
13 cyclohexane, methyl-	108-87-2	C7H14	98.19	727.945 , 1.010	1042597
14 pentane, 2,4-dimethyl-	108-08-7	C7H16	100.21	563.962 , 0.997	2235735
15 hexane, 2-methyl-	591-76-4	C7H16	100.21	627.955 , 0.983	4091529
16 heptane	142-82-5	C7H16	100.21	679.95 , 0.983	2828030
17 hexane, 2,5-dimethyl-	592-13-2	C8H18	114.23	731.945 , 0.970	171499
18 hexane, 2,4-dimethyl-	589-43-5	C8H18	114.23	735.944 , 0.977	361855
19 heptane, 2-methyl-	592-27-8	C8H18	114.23	783.94 , 0.977	3062274
20 octane	111-65-9	C8H18	114.23	831.935 , 0.977	1475688
21 octane, 4-methyl-	2216-34-4	C8H18	114.23	919.926 , 0.970	1434802
22 benzene, 1-propynyl-	673-32-5	C9H8	116.16	1183.9 , 1.624	476429
23 benzene, 2-propenyl-	300-57-2	C9H10	118.18	1107.91 , 1.320	1287879
24 indane	496-11-7	C9H10	118.18	1163.9 , 1.386	1484419
25 cumene	98-82-8	C9H12	120.20	1015.92 , 1.168	470608

26 benzene, propyl-	103-65-1	C9H12	120.20	1051.91 , 1.175	2371508
27 benzene, 1-ethyl-4-methyl-	622-96-8	C9H12	120.20	1063.91 , 1.175	11198299
28 benzene, 1,3,5-trimethyl-	108-67-8	C9H12	120.20	1079.91 , 1.181	8739518
29 benzene, 1-ethyl-3-methyl-	620-14-4	C9H12	120.20	1087.91 , 1.208	40890291
30 benzene, 1,2,4-trimethyl-	95-63-6	C9H12	120.20	1111.91 , 1.228	9924750
31 benzene, 1,2,3-trimethyl-	526-73-8	C9H12	120.20	1151.9 , 1.313	8119158
32 cis-1-ethyl-3-methyl-cyclohexane	19489-10-2	C9H18	126.24	967.921 , 0.997	1170929
33 pentane, 3-ethyl-2,2-dimethyl-	16747-32-3	C9H20	128.26	811.937 , 0.964	2051498
34 heptane, 3-ethyl-	15869-80-4	C9H20	128.26	931.925 , 0.970	673806
35 nonane	111-84-2	C9H20	128.26	963.922 , 0.977	2920704
36 naphthalene	91-20-3	C10H8	128.17	1407.88 , 2.125	3266024
37 benzene, 1-methyl-4-(1-methylethenyl)-	1195-32-0	C10H12	132.21	1223.9 , 1.426	2806451
38 1h-indene, 2,3-dihydro-5-methyl-	874-35-1	C10H12	132.21	1311.89 , 1.492	510063
39 1h-indene, 2,3-dihydro-4-methyl-	824-22-6	C10H12	132.21	1331.88 , 1.531	532061
40 dehydrosabinene	36262-09-6	C10H14	134.22	1055.91 , 1.096	5041122
41 2,6-dimethyl-1,3,5,7-octatetraene, E,E-	460-01-5	C10H14	134.22	1107.91 , 1.142	262692
42 benzene, 1-methyl-2-propyl-	1074-17-5	C10H14	134.22	1119.91 , 1.188	425289
43 <u>p-cymene</u>	99-87-6	C10H14	134.22	1135.9 , 1.201	2463619
44 benzene, 1-methyl-3-propyl-	1074-43-7	C10H14	134.22	1167.9 , 1.241	2631882
45 benzene, 2-ethyl-1,4-dimethyl-	1758-88-9	C10H14	134.22	1179.9 , 1.261	1273871
46 benzene, (1-methylpropyl)-	135-98-8	C10H14	134.22	1195.9 , 1.300	414454
47 benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	C10H14	134.22	1215.9 , 1.327	4877762
48 2,6-dimethyl-1,3,5,7-octatetraene, E,E-	460-01-5	C10H14	134.22	1251.89 , 1.346	493106
49 benzene, 1,2,3,5-tetramethyl-	527-53-7	C10H14	134.22	1283.89 , 1.406	1043097
50 cyclohexane, (1-methylpropyl)-	7058-01-7	C10H20	140.27	1139.9 , 1.049	547994
51 nonane, 3-methyl-	5911-04-6	C10H22	142.29	1011.92 , 0.970	322877
52 heptane, 3-ethyl-2-methyl-	14676-29-0	C10H22	142.29	1023.92 , 0.970	545020
53 nonane, 2-methyl-	871-83-0	C10H22	142.29	1043.91 , 0.970	4476777
54 decane	124-18-5	C10H22	142.29	1083.91 , 0.990	983016
55 naphthalene, 2-methyl-	91-57-6	C11H10	142.20	1587.86 , 2.178	999831
56 naphthalene, 1-methyl-	90-12-0	C11H10	142.20	1619.86 , 2.264	330941

57 naphthalene, 1,2,3,4-tetrahydro-6-methyl-	1680-51-9	C11H14	146.23	1511.87 , 1.630	418614
58 benzene, 1-methyl-4-(2-methylpropyl)-	5161-04-6	C11H16	148.25	1307.89 , 1.320	153268
59 benzene, pentyl-	538-68-1	C11H16	148.25	1315.89 , 1.327	394240
60 benzene, 1,3-diethyl-5-methyl-	2050-24-0	C11H16	148.25	1323.89 , 1.333	222656
61 decane, 2-methyl-	6975-98-0	C11H24	156.31	1159.9 , 1.003	3028633
62 decane, 3-methyl-	13151-34-3	C11H24	156.31	1171.9 , 1.003	519289
63 undecane	1120-21-4	C11H24	156.31	1203.9 , 1.023	2938931
64 decane, 2,9-dimethyl-	1002-17-1	C12H26	170.34	1295.89 , 1.036	1979016
65 dodecane	112-40-3	C12H26	170.34	1343.88 , 1.056	1612803
66 decane, 2,6,6-trimethyl-	62108-24-1	C13H28	184.37	1111.91 , 0.983	1416478
67 decane, 2,6,7-trimethyl-	62108-25-2	C13H28	184.37	1231.89 , 1.016	582331
68 tridecane	629-50-5	C13H28	184.37	1495.87 , 1.082	464008
69 tetradecane	629-59-4	C14H30	198.39	1655.85 , 1.102	681482
70 pentadecane	629-62-9	C15H32	212.42	1819.84 , 1.129	2586234
71 c16 isomer	n/a	C16H34	226.45	1831.83 , 1.069	391055
72 hexadecane	544-76-3	C16H34	226.45	1983.82 , 1.142	1130610
73 c17 isomer	n/a	C17H36	240.48	2071.81 , 1.122	424204
74 heptadecane	629-78-7	C17H36	240.48	2147.8 , 1.162	1648198
75 octadecane	593-45-3	C18H38	254.50	2319.79 , 1.228	921839
76 c19 isomer	n/a	C19H39	267.53	2347.78 , 1.195	317326
77 nonadecane	629-92-5	C19H40	268.53	2523.77 , 1.327	555457

alcohols, ketones, aldehydes, furans

78 acetone	67-64-1	C3H6O	58.08	347.983 , 1.492	187506473
79 furan	110-00-9	C4H4O	68.08	363.982 , 1.366	486951
80 methacrolein	78-85-3	C4H6O	70.09	467.971 , 1.406	430523
81 propanal, 2-methyl-	78-84-2	C4H8O	72.11	451.973 , 1.261	888470
82 2-butanone	78-93-3	C4H8O	72.11	507.967 , 1.379	6977405
83 furan, 2-methyl-	534-22-5	C5H6O	82.10	527.965 , 1.254	566928
84 furan, 3-methyl-	930-27-8	C5H6O	82.10	543.964 , 1.280	7453837
85 2-butenal, 3-methyl-	120-92-3	C5H8O	84.12	823.936 , 1.511	761582

86 butanal, 3-methyl-	590-86-3	C5H10O	86.13	611.957 , 1.241	1645900
87 butanal, 2-methyl-	96-17-3	C5H10O	86.13	627.955 , 1.214	645966
88 2-pentanone	107-87-9	C5H10O	86.13	663.952 , 1.280	977539
89 cyclopentanol	96-41-3	C5H10O	86.13	679.95 , 1.261	1255779
90 3-penten-2-one, 4-methyl-	141-79-7	C6H10O	98.15	843.934 , 1.307	217752
91 3-pentanone, 2-methyl-	565-69-5	C6H12O	100.16	767.941 , 1.175	930042
92 hexanal	66-25-1	C6H12O	100.16	835.934 , 1.221	1200340
93 2-heptanone	110-43-0	C7H14O	114.19	959.922 , 1.208	796755
94 2-heptanol	543-49-7	C7H16O	116.20	959.922 , 1.360	2784921
95 5-hepten-2-one, 6-methyl-	110-93-0	C8H14O	126.20	1075.91 , 1.261	3185093
96 1-octen-3-ol	3391-86-4	C8H16O	128.22	1059.91 , 1.399	372115
97 octanal	124-13-0	C8H16O	128.22	1095.91 , 1.201	2137337
98 1-octanol	111-87-5	C8H18O	130.23	1163.9 , 1.650	32837330
99 ethanone, 1-(4-methylphenyl)-	122-00-9	C9H10O	134.18	1383.88 , 2.224	1296295
100 2-nonanone	821-55-6	C9H18O	142.24	1207.9 , 1.320	768989
101 7-octen-2-ol, 2,6-dimethyl-	18479-58-8	C10H20O	156.27	1175.9 , 1.379	379122
102 decanal	112-31-2	C10H20O	156.27	1367.88 , 1.386	1101543

ethers, carboxylic acids, esters

103 acetic acid, methyl ester	79-20-9	C3H6O2	74.08	403.978 , 1.379	1107928
104 ethyl acetate	141-78-6	C4H8O2	88.11	539.964 , 1.267	6880992
105 2-propenoic acid, 2-methyl-, methyl ester	80-62-6	C5H8O2	100.12	703.948 , 1.254	1106236
106 2-butenoic acid, 2-methyl-, methyl ester	41725-90-0	C6H10O2	114.14	931.925 , 1.261	1625391
107 acetic acid, butyl ester	123-86-4	C6H12O2	116.16	851.933 , 1.168	226597
108 acetic acid, pentyl ester	628-63-7	C7H14O2	130.19	979.92 , 1.155	504216
109 propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3	74381-40-1	C8H14O3	158.20	2019.82 , 1.459	179994
110 2,6-octadienoic acid, 3,7-dimethyl-, methyl ester	2349-14-6	C11H18O2	182.26	1547.86 , 1.577	315333
111 2-decenoic acid, methyl ester, (e)-	7367-85-3	C11H20O2	184.28	1535.86 , 1.445	2007066
112 propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl es	74367-34-3	C12H24O3	216.32	1659.85 , 1.841	709172
113 octane, 1,1'-oxybis-	629-82-3	C16H34O	242.45	2087.81 , 1.234	577664

oxygenated aromatics

114 benzaldehyde	100-52-7	C7H6O	106.12	1067.91 , 1.742	3147759
115 3-hydroxyphenylacetylene	10401-11-3	C8H6O	118.14	1119.91 , 1.624	210162
116 benzeneacetaldehyde	122-78-1	C8H8O	120.15	1163.9 , 2.039	164767
117 acetophenone	98-86-2	C8H8O	120.15	1203.9 , 2.099	1991617

monoterpeneS

118 <u>α-pinene</u>	80-56-8	C10H16	136.24	1027.92 , 1.056	209247435
119 <u>α-phellandrene isomer</u>	n/a	C10H16	136.24	1031.91 , 1.109	235164599
120 <u>camphene</u>	79-92-5	C10H16	136.24	1047.91 , 1.056	102365
121 <u>myrcene</u>	123-35-3	C10H16	136.24	1075.91 , 1.076	519688220
122 <u>β-pinene</u>	127-91-3	C10H16	136.24	1083.91 , 1.129	447295616
123 <u>α-phellandrene</u>	99-83-2	C10H16	136.24	1111.91 , 1.102	6821046
124 <u>δ^3-carene</u>	13466-78-9	C10H16	136.24	1115.91 , 1.115	89252
125 <u>limonene</u>	138-86-3	C10H16	136.24	1139.9 , 1.135	111634319
126 <u>β-phellandrene</u>	555-10-2	C10H16	136.24	1147.9 , 1.155	182984266
127 <u>γ-terpinene</u>	99-85-4	C10H16	136.24	1171.9 , 1.168	3132837
128 <u>terpinolene</u>	586-62-9	C10H16	136.24	1211.9 , 1.214	8717506

oxygenated monoterpeneS

129 bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-	18358-53-7	C10H16O	152.24	1371.88 , 1.610	1999009
130 <u>4-terpinenol</u>	562-74-3	C10H18O	154.25	1351.88 , 1.630	2075482
131 <u>terpineol</u>	98-55-5	C10H18O	154.25	1371.88 , 1.815	1054362

sesquiterpeneS

132 <u>α-cubebene</u>	17699-14-8	C15H24	204.36	1623.86 , 1.221	296641
133 <u>α-longipinene</u>	5989-08-2	C15H24	204.36	1659.85 , 1.267	2615092
134 <u>copaene</u>	3856-25-5	C15H24	204.36	1683.85 , 1.261	10195649
135 <u>β-bourbonene</u>	5208-59-3	C15H24	204.36	1707.85 , 1.287	679995
136 <u>α-cedrene</u>	469-61-4	C15H24	204.36	1771.84 , 1.356	10065235
137 <u>caryophyllene</u>	87-44-5	C15H24	204.36	1775.84 , 1.360	17713723
138 <u>humulene</u>	6753-98-6	C15H24	204.36	1835.83 , 1.426	2583753
139 <u>(Z,E)-α-farnesene</u>	26560-14-5	C15H24	204.36	1883.83 , 1.399	2293128
140 <u>δ-cadinene</u>	483-76-1	C15H24	204.36	1911.83 , 1.439	1255593

S-, or N-containing

141	disulfide, dimethyl	624-92-0	C2H6S2	94.20	763.942 , 1.346	751263
142	pentanenitrile, 4-methyl-	542-54-1	C6H11N	97.16	899.928 , 1.432	386760

142 total number of compounds meeting the peak selection criteria

15 compounds positively identified

127 compounds tentatively identified