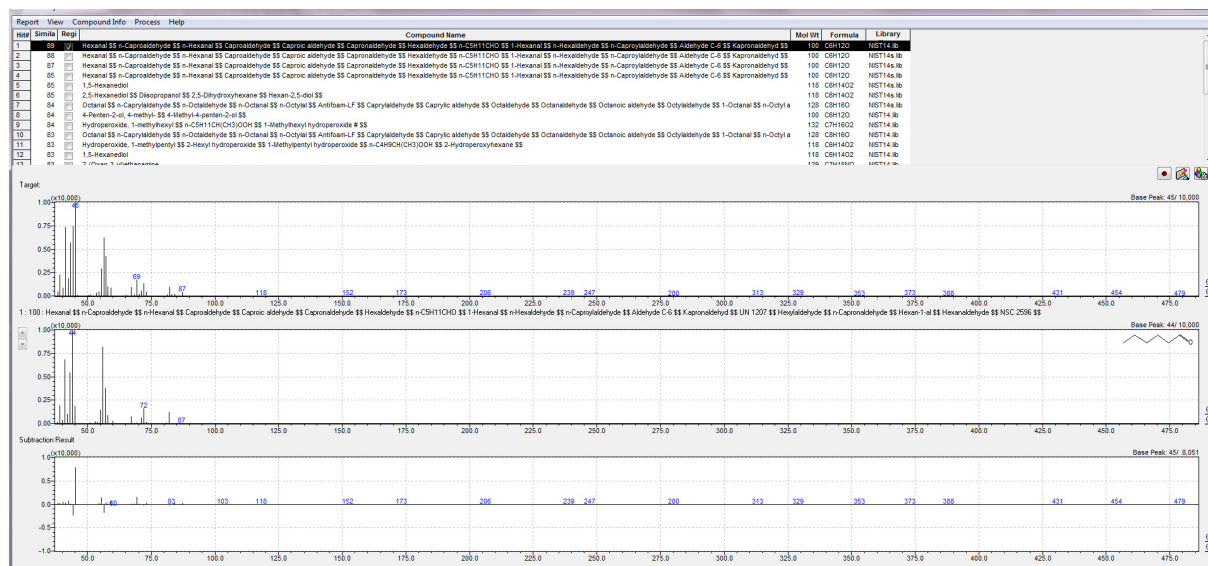


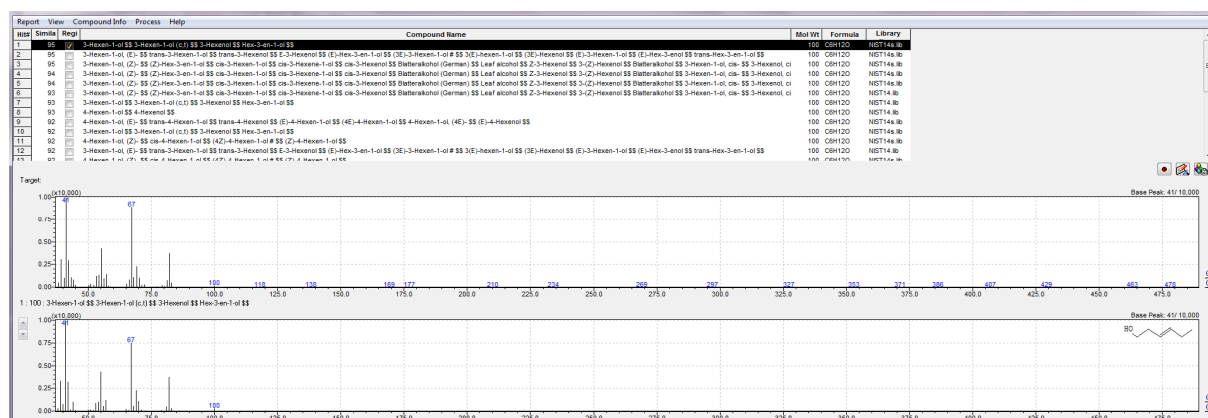
Supplementary Material S1. Comparison of the identified organic compounds (VOCs) with the mass spectral library.

Numbers 1-18 correspond with Table 1.

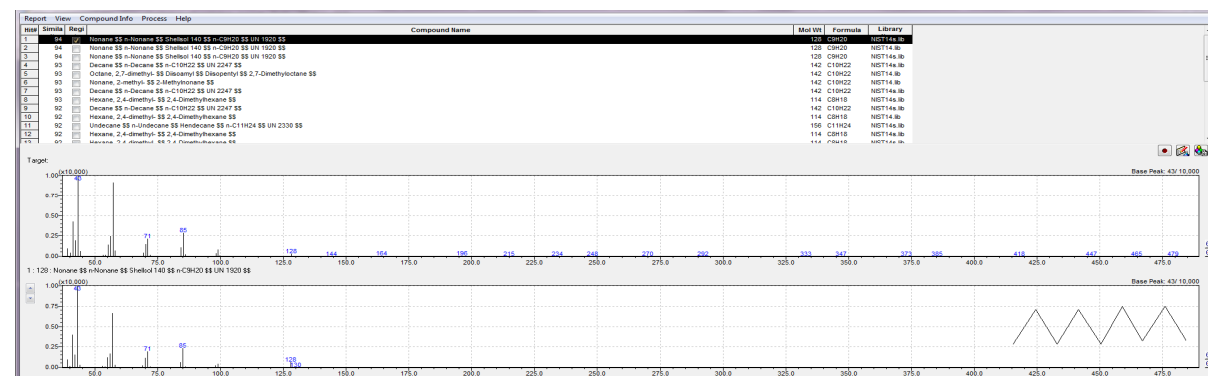
1.



2.



3.



[illegible][illegible][illegible]

[illegible]

Report View Compound Info Process Help				Compound Name			Mol Wt	Formula	Library
Item	Similar	Reg							
1	95	95	Decane S5 n-Decane S5 n-C19H22 S5 UN 2247 S5				142	C19H22	NIST14a.lb
2	95		Undecane S5 n-Undecane S5 Hendecane S5 n-C11H24 S5 UN 2330 S5				158	C11H24	NIST14a.lb
3	94		Decane S5 n-Decane S5 n-C19H22 S5 UN 2247 S5				142	C19H22	NIST14a.lb
4	94		Undecane S5 n-Undecane S5 Hendecane S5 n-C11H24 S5 UN 2330 S5				158	C11H24	NIST14a.lb
5	94		Decane S5 n-Decane S5 n-C19H22 S5 UN 2247 S5				142	C19H22	NIST14a.lb
6	94		Tridecane S5 n-Tridecane S5 Tridecane n S5				184	C13H28	NIST14a.lb
7	93		Decane S5 n-Decane S5 n-C19H22 S5 UN 2247 S5				142	C19H22	NIST14a.lb
8	93		Undecane S5 n-Undecane S5 Hendecane S5 n-C11H24 S5 UN 2330 S5				158	C11H24	NIST14a.lb
9	93		Dodecane S5 n-Dodecane S5 Asakane 12 S5 Da 51-290453 S5 CH3(CH2)10CH3 S5 Dihexyl S5 Dihexyl S5 Duodecane S5 NSC 8714 S5				170	C12H26	NIST14a.lb
10	93		Undecane S5 n-Undecane S5 Hendecane S5 n-C11H24 S5 UN 2330 S5				158	C11H24	NIST14a.lb
11	93		Undecane 2,10-dimethyl S5 2,10-Dimethylundecane S5 S5				184	C13H28	NIST14a.lb
12	93		Octane 4-ethyl S5 4-EthylOctane S5				142	C10H22	NIST14a.lb
13	93		Dodecane S5 n-Dodecane S5 Asakane 12 S5 Da 51-290453 S5 CH3(CH2)10CH3 S5 Dihexyl S5 Dihexyl S5 Duodecane S5 NSC 8714 S5				170	C12H26	NIST14a.lb

[illegible]

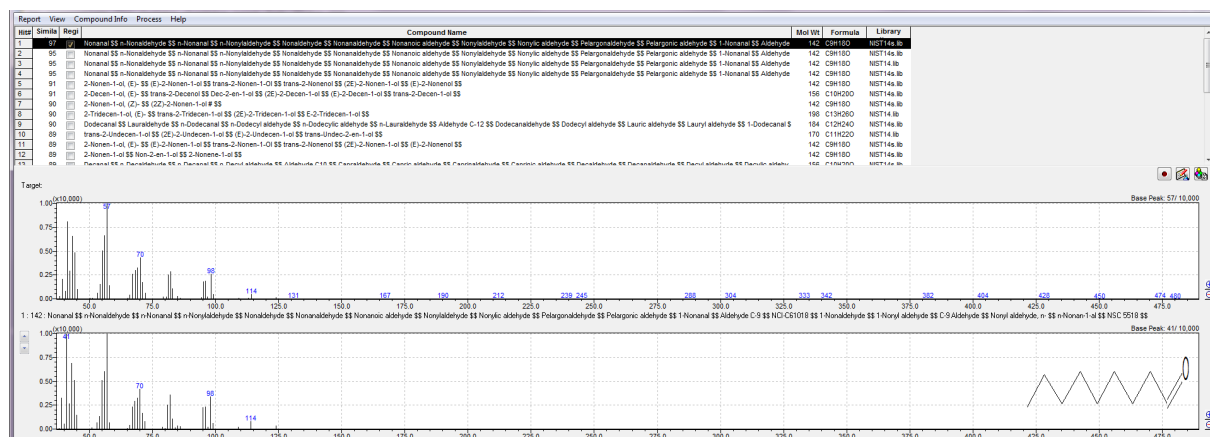
Report View	Compound Info	Process Help
Real Time Data	Compound Name	Mat Ut
1	92 D-Limonene S5 Cyclohexene, 1-methyl-4-(1-methylethyl), (R)- S5 p-Menth-1,8-diene, (R)- S5 (+)-[R]-Limonene S5 (+)-[4R]-Limonene S5 (+)-p-Menth-1,8-diene S5 (+)-Limonene S5 (R)- S5 (+)-Limonene S5 Carvone S5 D-(-)-Limo	136 C10H16
2	92 D-Limonene S5 Cyclohexene, 1-methyl-4-(1-methylethyl), (R)- S5 p-Menth-1,8-diene, (R)- S5 (+)-[R]-Limonene S5 (+)-[4R]-Limonene S5 (+)-p-Menth-1,8-diene S5 (+)-Limonene S5 (R)- S5 (+)-Limonene S5 Carvone S5 D-(-)-Limo	136 C10H16
3	92 D-Limonene S5 Cyclohexene, 1-methyl-4-(1-methylethyl), (R)- S5 p-Menth-1,8-diene, (R)- S5 (+)-[R]-Limonene S5 (+)-[4R]-Limonene S5 (+)-p-Menth-1,8-diene S5 (+)-Limonene S5 (R)- S5 (+)-Limonene S5 Carvone S5 D-(-)-Limo	136 C10H16
4	92 Cyclohexene, 1-methyl-4-(1-methylethyl), (S)- S5 p-Menth-1,8-diene, (S)- S5 (+)-Limonene S5 Limonene S5 Limonene S5 4-isopropenyl-1-methyl-1-cyclohexene # S5	136 C10H16
5	92 Cyclohexene, 1-methyl-4-(1-methylethyl), (S)- S5 p-Menth-1,8-diene, (S)- S5 (+)-Limonene S5 Caputene S5 Caputene S5 Cinen S5 Cinen S5 Dipentene S5 Dipentene S5 Eulimen S5 Kaudoen S5 Limonen S5 Neosol S5 p-Men	136 C10H16
6	92 Cyclohexene, 1-methyl-4-(1-methylethyl), (S)- S5 p-Menth-1,8-diene, (S)- S5 (+)-Limonene S5 Limonene S5 Limonene S5 4-isopropenyl-1-methyl-1-cyclohexene # S5	136 C10H16
7	91 Cyclobutane, 1,2-bis(1-methylethyl), trans- S5 1,2-Diisopropenylcyclobutane # S5	136 C10H16
8	91 Cyclohexene, 1-methyl-4-(1-methylethyl), (S)- S5 p-Menth-1,8-diene, (S)- S5 (+)-Limonene S5 Limonene S5 Limonene S5 4-isopropenyl-1-methyl-1-cyclohexene # S5	136 C10H16
9	90 Cyclobutane, 1,2-diisopropenyl, trans S5 1,2-Diisopropenylcyclobutane # S5	136 C10H16
10	90 Limonene S5 Cyclohexene, 1-methyl-4-(1-methylethyl), (S)- S5 p-Menth-1,8-diene, (S)- S5 (+)-Limonene S5 Caputene S5 Caputene S5 Cinen S5 Cinen S5 Dipentene S5 Dipentene S5 Eulimen S5 Kaudoen S5 Limonen S5 Neosol S5 p-Men	136 C10H16
11	90 Cyclohexanol, 1-methyl-4-(1-methylethyl), acetate S5 p-Menth-1,8-diene, (S)- S5 (+)-Limonene S5 Limonene S5 Limonene S5 4-isopropenyl-1-methyl-1-cyclohexene # S5	136 C10H16
12	90 Cyclohexanol, 1-methyl-4-(1-methylethyl), S5 4-isopropenyl-1-methyl-1-cyclohexene # S5	136 C10H16
13	90 Cyclohexene, 1-methyl-4-(1-methylethyl), (R)- S5 p-Menth-1,8-diene, (R)- S5 (+)-[R]-Limonene S5 (+)-[4R]-Limonene S5 (+)-p-Menth-1,8-diene S5 (+)-Limonene S5 (R)- S5 (+)-Limonene S5 Carvone S5 D-(-)-Limo	136 C10H16

Target

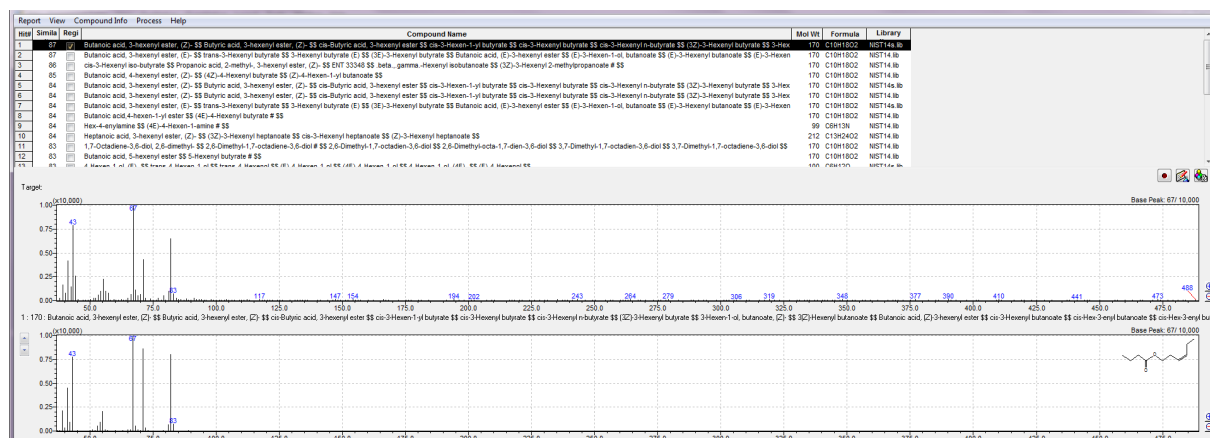
1: 136 D-Limonene S5 Cyclohexene, 1-methyl-4-(1-methylethyl), (R)- S5 p-Menth-1,8-diene, (R)- S5 (+)-[R]-Limonene S5 (+)-[4R]-Limonene S5 (+)-p-Menth-1,8-diene S5 (+)-Limonene S5 (R)- S5 (+)-Limonene S5 Carvone S5 D-(-)-Limonene, [D]- S5 Limonene, [L]- S5 (R)- 1-methyl-4-(1-methylethyl)cyclohexane S5 Dextro limonene S5 (R)- 4-isopropenyl-1-methyl-1-cyclohexene S5 4-isopropenyl-1-methyl-1-cyclohexene S5

[illegible][illegible]

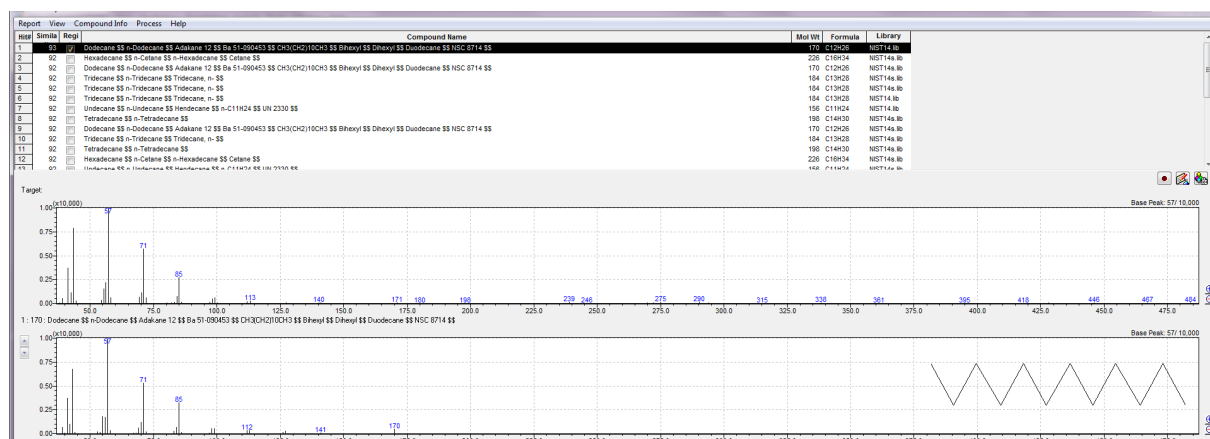
13.



14.



15.



Report	View	Compound Info	Process	Help	
1	Table	Compound Name	Mol Wt	Formula	Library
1	62	cis-3-Hexenyl alpha-methylbutyrate S\$ Butanoic acid, 2-methyl-, 3-hexenyl ester, (Z)- S\$ (3Z)-3-Hexenyl 2-methylbutanoate # \$S	164	C11H20O2	NIST14a.lb
2	92	n-Valeric acid cis-3-hexenyl ester S\$ cis-3-Hexenyl valerate S\$ Pentanoic acid, 3-hexenyl ester, (Z)- S\$ cis-3-Hexenyl n-valerate S\$ (Z)-3-Hexenyl-1-oil, pentanoate S\$ (Z)-3-Hexenyl pentanoate S\$ (Z)-3-	164	C11H20O2	NIST14a.lb
3	92	cis-3-Hexenyl alpha-methylbutyrate S\$ Butanoic acid, 2-methyl-, 3-hexenyl ester, (Z)- S\$ (3Z)-3-Hexenyl 2-methylbutanoate # \$S	164	C11H20O2	NIST14a.lb
4	92	Pentanoic acid, 4-hexen-1-yl ester S\$ (E)-4-Hexenyl pentanoate # \$S	164	C11H20O2	NIST14a.lb
5	90	cis-3-Hexenyl isovalerate S\$ Isovaleric acid cis-3-hexenyl ester S\$ Butanoic acid, 3-methyl-, 3-hexenyl ester, (Z)- S\$ AD-35966 S\$ cis-3-Hexenyl 3-methylbutanoate S\$ cis-3-Hexenyl iso-valer	164	C11H20O2	NIST14a.lb
6	90	Formic acid, cyclohexyl ester S\$ Cyclohexyl formate S\$ Cyclohexyl ester of formic acid S\$ Formic acid, cyclohexyl ester (purified) S\$	133	C7H12O2	NIST14a.lb
7	89	cis-3-Hexenyl isovalerate S\$ Isovaleric acid cis-3-hexenyl ester S\$ Butanoic acid, 3-methyl-, 3-hexenyl ester, (Z)- S\$ AD-35966 S\$ cis-3-Hexenyl 3-methylbutanoate S\$ cis-3-Hexenyl iso-valer	164	C11H20O2	NIST14a.lb
8	89	cis-3-Hexenyl isovalerate S\$ Isovaleric acid cis-3-hexenyl ester S\$ Butanoic acid, 3-methyl-, 3-hexenyl ester, (Z)- S\$ AD-35966 S\$ cis-3-Hexenyl 3-methylbutanoate S\$ cis-3-Hexenyl iso-valer	164	C11H20O2	NIST14a.lb
9	89	Formic acid, cyclohexyl ester S\$ Cyclohexyl formate S\$ Cyclohexyl ester of formic acid S\$ Formic acid, cyclohexyl ester (purified) S\$	133	C7H12O2	NIST14a.lb
10	88	cis-3-Hexenyl isovalerate S\$ Isovaleric acid cis-3-hexenyl ester S\$ Butanoic acid, 3-methyl-, 3-hexenyl ester, (Z)- S\$ AD-35966 S\$ cis-3-Hexenyl 3-methylbutanoate S\$ cis-3-Hexenyl iso-valer	164	C11H20O2	NIST14a.lb
11	88	n-Valeric acid cis-3-hexenyl ester S\$ cis-3-Hexenyl valerate S\$ Pentanoic acid, 3-hexenyl ester, (Z)- S\$ cis-3-Hexenyl n-valerate S\$ (Z)-3-Hexenyl-1-oil, pentanoate S\$ (Z)-3-Hexenyl pentanoate S\$ (Z)-3-	164	C11H20O2	NIST14a.lb
12	87	Pentanoic acid, 4-hexen-1-yl ester S\$ (E)-4-Hexenyl pentanoate # \$S	165	C11H20O2	NIST14a.lb
13	87	1 Hexenyl 3-ol isomerase, (P); 6E Hexenyl 3-ol isomerase, (P); 6E hex-3-enal; Hexenyl isomerase 6E cis-3 Hexenyl isomerase 6E Dimeric acid cis-3 Hexenyl ester 6E beta, gamma Hexenyl isomerase cis-6E cis-3 Hexenyl 6-ol	165	C10H18O2	NIST14a.lb

Target

Base Peak: 671.1000

1: 184: cis-3-Hexenyl alpha-methylbutyrate S\$ Butanoic acid, 2-methyl-, 3-hexenyl ester, (Z)- S\$ (3Z)-3-Hexenyl 2-methylbutanoate # \$S

Base Peak: 671.1000

CCCCC/C=C\CCCC(=O)OC(C)CC

Report View Compound Info Process Help

Rank	Similarity	Regio	Compound Name	Mol Wt	Formula	Library
1	91	(Z)-[2-Hex-3-en-1-yl 2-methylbut-2-enoate] \$S\$ 2-Butenic acid, 2-methyl-, (Z)-; 3-Hexen-1-yl ester-, (Z)-; \$S\$ 2-Butenic acid, 2-methyl-, (Z)-; 3-Hexenyl ester-, (Z)-; (Z)-3-Hexenyl 2-methylbut-2-enoate	162	C ₁₁ H ₁₈ O ₂	NIST14a	
2	88	(Z)-Hex-3-enyl (E)-2-methylbut-2-enoate	162	C ₁₁ H ₁₈ O ₂	NIST14a	
3	88	Hexenyl angolate, 4Z	162	C ₁₁ H ₁₈ O ₂	NIST14a	
4	88	(E)-Hex-3-enyl (E)-2-methylbut-2-enoate	162	C ₁₁ H ₁₈ O ₂	NIST14a	
5	87	Hexenyl ligate, 4Z	162	C ₁₁ H ₁₈ O ₂	NIST14a	
6	84	Cyclohexane, 3-propenyl- \$S\$ Cyclohexane, allyl- \$S\$ Allylcyclohexane \$S\$ 1-Cyclohexyl-2-propene \$S\$ 1-Propene, 3-cyclohexyl- \$S\$ 3-Cyclohexyl-1-propene \$S\$ Acetic acid, trifluoro-, cyclohexyl ester \$S\$ Trifluoroacetic acid, cyclohexyl ester \$S\$ Cyclohexyl trifluoroacetate \$S\$ \$S\$	124	C ₈ H ₁₆	NIST14a	
7	84	Cyclohexane, chloro- \$S\$ Chlorocyclohexane \$S\$ Cyclohexyl chloride \$S\$ Monochlorocyclohexane \$S\$	116	C ₆ H ₁₁ Cl	NIST14a	
8	83	Cyclohexane, chloro- \$S\$ Chlorocyclohexane \$S\$ Cyclohexyl chloride \$S\$ Monochlorocyclohexane \$S\$	116	C ₆ H ₁₁ Cl	NIST14a	
9	83	Cyclohexane, (1-methylallyl)- \$S\$ Cyclohexane, isopropyl- \$S\$ Isopropylcyclohexane \$S\$ Neohydrocyclohexane \$S\$ Norhamthane \$S\$	126	C ₉ H ₁₈	NIST14a	
10	83	Cyclohexane, 2-propenyl- \$S\$ Cyclohexane, allyl- \$S\$ Allylcyclohexane \$S\$ 1-Cyclohexyl-2-propene \$S\$ 1-Propene, 3-cyclohexyl- \$S\$ 3-Cyclohexyl-1-propene \$S\$	124	C ₈ H ₁₆	NIST14a	
11	83	Vinylcyclohexyl ether \$S\$ Cyclohexane, (ethenyl)- \$S\$ Vinylcyclohexane \$S\$ \$S\$	126	C ₈ H ₁₆ O	NIST14a	
12	83	Cyclohexane, 1-methyl- \$S\$ Cyclohexane, ethyl- \$S\$ Ethylcyclohexane \$S\$ 1-Cyclohexyl-1-methane \$S\$ 1-Methane, 3-cyclohexyl- \$S\$ 3-Cyclohexyl-1-methane \$S\$	114	C ₈ H ₁₆	NIST14a	

Target

Base Peak: 671.10000

1: 182: (Z)-[2-Hex-3-en-1-yl 2-methylbut-2-enoate] \$S\$ 2-Butenic acid, 2-methyl-, (Z)-; 3-Hexen-1-yl ester-, (Z)-; \$S\$ 2-Butenic acid, 2-methyl-, (Z)-; 3-Hexenyl ester-, (Z)-; (Z)-3-Hexenyl 2-methylbut-2-enoate \$S\$

Base Peak: 821.10000

[illegible]

Supplementary material S2. The description of ecological indices used for data analysis.

The **dominance index (d)** of each species was calculated according to the formula:

$$d = \frac{n_i}{N}$$

where n_i is the abundance of individuals belonging to the i th taxa and N – the total abundance of all taxa.

The **Berger-Parker dominance index (D)** was calculated according to the formula:

$$D = \frac{n_{max}}{N}$$

where n_{max} is the abundance of the most abundant species taxa and N – is the total abundance of all taxa.

The **Shannon-Weaver (H')** index was calculated according to the following formula:

$$H' = - \sum_{i=1}^R p_i \ln p_i$$

where p_i is the proportion of individuals belonging to the i th taxa.

The **Pielou (J)** index was calculated according to the formula:

$$J = \frac{H'}{\ln(S)}$$

where H' is the Shannon-Weaver index and S is the total number of species in a sample.

The **Margalef's species richness (S)** index was calculated according to the following formula:

$$S = \frac{s - 1}{\ln(N)}$$

where s is the total number of species in a sample and N the total number of individuals in the sample.

The **species stability (C)** was calculated according to the following formula:

$$C = 200 \frac{n_a}{N}$$

where n_a is the total number of samples with species and N is the total number of samples.

The **Jaccard similarity index (SJ)** was calculated according to the formula:

$$SJ = \frac{c}{a + b + c}$$

where c is the number of shared species between the two sites and a and b are the number of species unique to each site.

References

- Berger, W.H., Parker F.L. Diversity of Planktonic Foraminifera in Deep Sea Sediments. *Science* **1970**, 168, 1345. <https://doi.org/10.1126/science.168.3937.1345>.
- Shannon, C.E. A Mathematical Theory of Communication. *Bell Syst. Tech. J.* **1948**, 27, 379-423. <https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>
- Pielou, E.C. The measurement of diversity in different types of biological collections. *J. Theor. Biol.* **1966**, 13, 131-144. [https://doi.org/10.1016/0022-5193\(66\)90013-0](https://doi.org/10.1016/0022-5193(66)90013-0)
- Margalef, R., Information Theory in Ecology. *General Systems* **1958**, 3, 36-71.
- Trojan, P. *General Ecology (Ekologia ogólna)*; PWN Publishing: Warsaw, Poland, 1980.
- Jaccard, P. The Distribution of the Flora of the Alpine Zone. *New Phytologist* **1912**, 11, 37-50. <http://dx.doi.org/10.1111/j.1469-8137.1912.tb05611.x>