

Supplementary

S1 Gas concentration approximation

- a. Maximum limit based on the assumption that the liquid drop was fully evaporated

We can approximate the amount of the vapor due to vapor pressure based on the equation expressed in previous question.

$$n_{VOC} = \frac{P_{VOC}V_{Total}}{RT}$$

From the evaporated amount from 5 μ l each reagent drops, we can finally approximate the concentration when it will be fully evaporated.

$$C_{VOC,max}[ppmv] = \frac{\frac{P_{VOC}}{P_{atm}} \times 10^6 \times V_{total\ reagent}}{n_{VOC} \times \frac{Molar\ mass}{Density}} = \frac{RT \times 10^6 \times V_{total\ reagent}}{V_{Total} \times \frac{Molar\ mass}{Density}}$$

VOC	Amount (mole)	Density (g/ml)	Molar mass (g/mol)	$C_{VOC,max}$ [ppmv]
Linalool	1.08 X 10 ⁻⁶	0.86	154.25	5683
Cis-3-hexen-1-ol	5.89 X 10 ⁻⁶	0.846	100.159	8610
Cis-3-hexenyl-acetate	7.85 X 10 ⁻⁶	0.897	142.198	6430
Methyl salicylate	2.2 X 10 ⁻⁷	1.174	152.149	7865

Table S 1. Maximum concentration limit for each VOC

- b. Approximation of mixture concentration

$$Concentration = Volume\ percent\ ratio \times Density_{Mixture} \times 10^6 \left(\frac{mg}{L} = \frac{\mu g}{ml} \right)$$

$$Density_{Mixture} = \frac{Density_{Linalool} + Density_{Cis-3-hexen-1-ol} + Density_{Methyl\ salicylate}}{3}$$

	Average GC/MS peak area		Recovery (%)
	Standard	VOC eluate	
Linalool	90285570	87460823	97
<i>cis</i> -3-Hexen-1-ol	65759826	56046591	85
<i>cis</i> -3-Hexenyl acetate	67767688	66787699	98
Methyl salicylate	61623426	22858992	37

Table S 2. Recovery rate comparison according to the tested VOCs

Wavenumber (cm ⁻¹)	LI vs. MIX	HA vs. MIX	HO vs. MIX	MS vs. MIX
808	0.84	0.83	0.83	0.60
812	0.86	0.85	0.83	0.70
1032	0.95	0.94	0.93	0.79
1040	0.86	0.78	0.79	0.74
1644	0.77	0.88	0.85	0.83
1652	0.81	0.82	0.73	0.82
1656	0.86	0.86	0.88	0.86
1672	0.45	0.88	0.86	0.83

Table S 3. Loading matrix of PC 1 for the case study (VOC vs. Mixture)

PC number	Eigenvalue	Percent (%)	Cumulative percentage (%)
1	2.9477	42.110	42.110
2	1.4194	20.276	62.386
3	0.9911	14.159	76.545
4	0.8430	12.043	88.588
5	0.3864	5.520	94.108
6	0.2646	3.780	97.888
7	0.1479	2.112	100.000

Table S 4. Cumulative percentage of PC of mixture for PCR

Wavenumber (cm^{-1})	PC 1	PC 2
808	0.8244	0.2459
812	0.9086	0.1640
1032	0.8879	-0.1987
1644	0.2518	0.8721
1656	0.5740	-0.5649
1676	0.3075	0.2685
1680	0.4085	-0.3750

Table S 5. Loading matrix of PC 1 and PC 2 of mixture for PCR

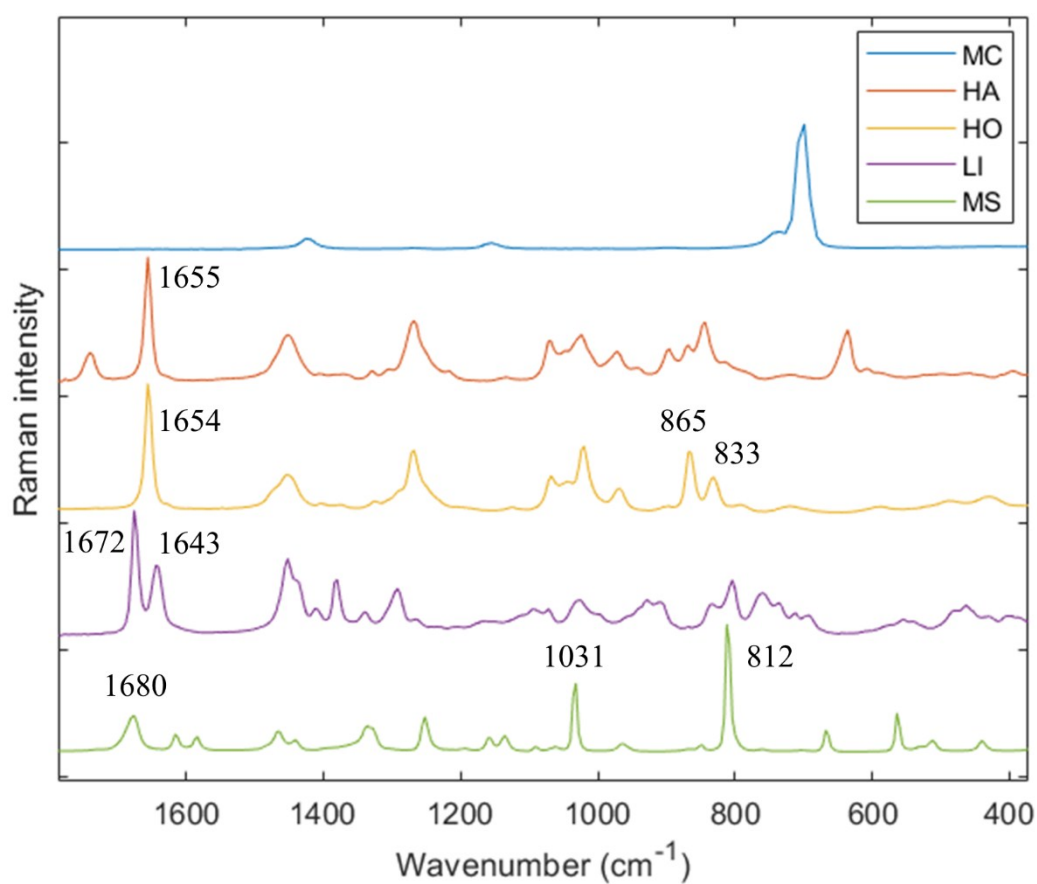


Figure S 1. Raman spectra for four standards

(MC: dichloromethane, HA: cis-3-hexenyl acetate, HO: cis-3-hexen-1-ol, LI: linalool, MS: methyl salicylate)

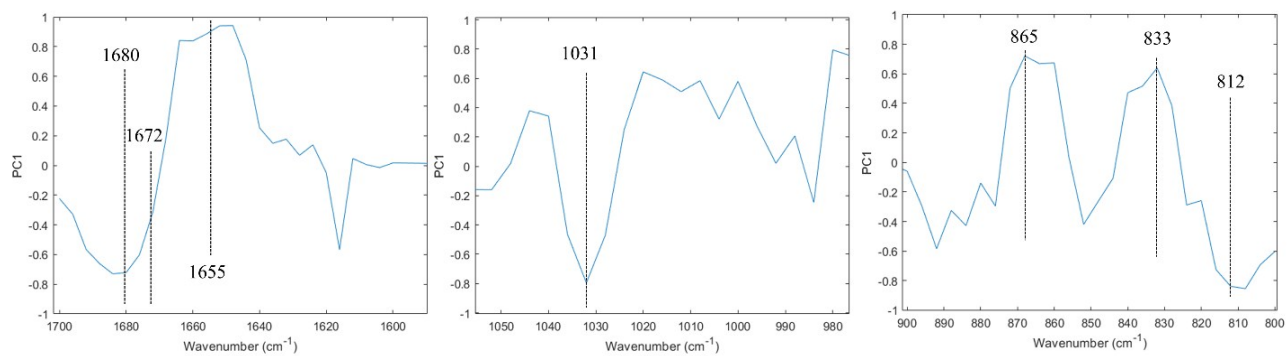


Figure S 2. Plot of PC 1 versus identified wavenumbers

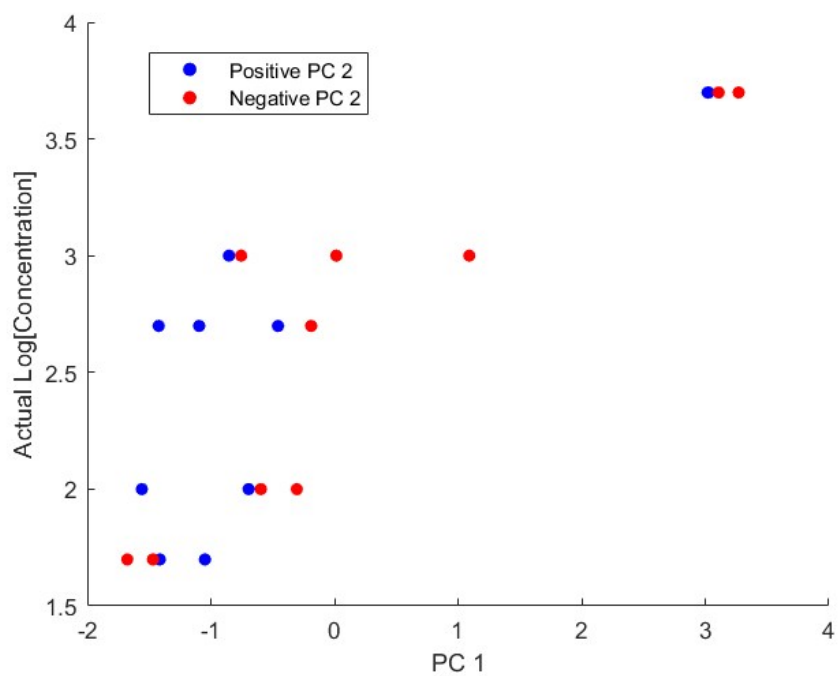


Figure S 3. Plot of PC 1 versus concentration according to the sign of PC 2