Supplemental Information

Ammonium-adduct chemical ionization to investigate anthropogenic oxygenated gas-phase organic compounds in urban air

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S1. Detailed description of correlations observed between trends in measured ions

To supplement the discussion in the main text and accompany correlation-related figures S9-12, here we use both concentration and ion abundance-based linear regressions to compare correlations between oxygenated species that potentially have similar or co-located sources. Only ions with the strongest correlations ranging from 0.85 to 1 were considered here to reduce the effect of meteorological influences on linear regressions. Compounds are also identified whose dynamics in the atmosphere could be important from an emissions or air quality perspective and warrant further investigation in future studies. Given that a wide range of possible uses exist for many of these compounds, mentions of specific sources are not intended to exclude other potential contributing source types, but rather to identify co-varying compounds (and shared uses) where potentially useful to the reader.

Glycols and glycol ethers

$C_2H_6O_2$, a prominent ion in this study identified primarily as ethylene glycol, showed very good correlations ($r > 0.9$) with 19 other ions, and was most strongly correlated ($r > 0.95$) with C_3H_9NO (e.g. aminopropanol). Most of these were volatile C_xH_yO ions with carbon numbers ≤ 6 including C_3H_6O (e.g. acetone), C_4H_6O (e.g. MVK), $C_6H_{10}O$ (e.g. cyclohexanone) and C_5H_8O (e.g. cyclopentanone), but also $C_{10}H_{12}O$ (e.g. benzyl acetone) and among others. The remaining ones were largely ester-containing $C_xH_yO_2$ ions. These compounds are widely used as solvents, with some also likely constituents of personal care products. This suggested that solvents could be an important contributor of $C_2H_6O_2$ in ambient environments.

Glycol ether-related ions generally did not show very strong correlations with other ions. With the exception of $C_8H_{18}O_2$ (e.g. EGHE) and $C_8H_{18}O_3$ (e.g. dipropylene glycol butyl ether or DGBE), almost all ions in this category were correlated with $r \leq 0.9$. EGHE is used in many consumer and commercial products while DGBE is a popular solvent. The strongest correlations ($r > 0.95$) of $C_8H_{18}O_2$ were with ions representing menthol, linalool and benzyl acetate, which was consistent with the popular use of EGHE in fragrance-related products. EGHE also showed good correlations ($r > 0.9$) with 29 other ions that were mainly constituted by C_xH_yO and $C_xH_yO_4$ ion groups such as C_7H_8O, $C_{11}H_{20}O$, $C_{14}H_{22}O$, $C_{16}H_{30}O_4$, $C_{10}H_{22}O_4$ and $C_9H_{18}O_4$. In the case of DGBE, no ions showed $r > 0.95$ but 17 ions were well-correlated ($r > 0.9$). The highest of these were ions containing EGHE, benzyl alcohol and some oxy-terpenoids such as menthol and linalool.

$C_6H_{12}O_3$ likely included propylene glycol methyl ether acetate (PGMEA) and 2-ethoxyethyl acetate that are widely used in coatings, printing inks and cleaning products. However, only 3 other ions correlated well ($r > 0.9$) with $C_6H_{12}O_3$. These included $C_7H_{14}O_3$ (e.g. ethyl-3-ethoxypropionate), $C_8H_{16}O_3$ (e.g. butoxyethyl acetate) and $C_6H_{12}O$ (e.g. methyl butyl ketone) while another 33 ions showed an $r > 0.85$. The highest among these remaining ones were C_xH_yO ions containing acetone, MVK and benzyl acetone.

Select personal care product-related compounds

Personal care products also likely contributed to glycol ether-related ion measurements. For example, $C_8H_{10}O_2$ (e.g. phenoxyethanol) was well-correlated ($r > 0.9$) with C_7H_8O, $C_{10}H_{12}O$, $C_{10}H_{18}O$ and $C_{10}H_{20}O$ ions, which represent benzyl alcohol, benzyl acetone, menthol and linalool. This was consistent with two major contributing isomers to $C_8H_{10}O_2$ being phenoxyethanol and 1,4 dimethoxybenzene that are used in personal care products. The isomer contributions were further substantiated by $C_8H_{10}O_2$ concentration peaks that coincided with morning and evening commute hours. Among other species in this category, $C_{10}H_{22}O_4$ (e.g. triethylene glycol butyl ether or TEGBE) most strongly correlated with $C_{14}H_{22}O$ (e.g. α-isomethyl ionone) ($r > 0.95$) that is primarily used in perfumes and other cosmetic products. Other major correlations included ions containing EGHE and benzyl acetate ($r > 0.9$).

Carbonyls

Ions representing carbonyls also showed good correlations with a wide range of ions. C_3H_6O (e.g. acetone) exhibited strong correlations ($r > 0.95$) with C_3H_9NO (e.g. aminopropanol), $C_6H_{10}O$ (e.g. cyclohexanone) and $C_8H_{14}O$ (6-methyl-5-hepten-2-one). However, it was also well-correlated ($r > 0.9$) with 30 more ions that were dominated by C_xH_yO compounds with $C_{\#}$'s ranging from 4 to 12 such as MVK, MEK, cyclopentanone, and benzyl acetone. In addition, $C_xH_yO_2$ ions related to cyclohexyl acetate, ethyl acetoacetate, ethylene glycol and butyl acrylate were also well-correlated with acetone. $C_6H_{10}O$ (e.g. cyclohexanone) correlated strongly with $C_4H_6O_2$, C_5H_8O and $C_8H_{14}O_2$ ions consistent with the popular use of cyclohexanone as a general solvent. $C_6H_{10}O$ also correlated well with $C_8H_{16}O$, $C_{10}H_{12}O$ and $C_6H_{10}O_2$ ions that are related to personal care products.

C_4H_8O (e.g. MEK) exhibited particularly strong correlations ($r > 0.95$) with ions prevalent in oxygenated solvents suggesting connections to solvent-related sources. There likely were smaller contributions from personal care products as evidenced by good correlations with C_3H_9NO, $C_6H_{10}O$, $C_6H_{12}O$ and $C_8H_{14}O$. Other carbonyl-related ions (e.g. $C_6H_{12}O$) were mainly strongly correlated with compounds used in fragrances and cosmetic products. C_7H_6O (e.g. benzaldehyde) showed strongest correlation with C_8H_8O (e.g. acetophenone) which is used in solvents and fragrances but also found in automobile exhaust. It also varied strongly with $C_6H_{12}O$, $C_8H_{16}O$, $C_{10}H_{12}O$ and $C_9H_{10}O_2$ that suggest solvents and cosmetics to be major sources. Overall, this supports large contributions of solvent-related sources to carbonyl-related ions.

Some variability was observed in the number of species with which the oxy-terpenoid-related ions were strongly correlated, suggestive of multiple sources types. For example, $C_{10}H_{20}O$ (e.g. menthol) showed good correlations ($r > 0.9$) with 41 ions. Of these, 14 ions were strongly correlated (r > 0.95) and included glycol ethers, carbonyls, esters and alcohols. $C_{10}H_{18}O$ correlated nearly perfectly with $C_{10}H_{20}O$. On the other hand, $C_{10}H_{16}O$ (e.g. camphor) was well-correlated (r > 0.9) with only four ions that included other major oxy-terpenoid-related ions, i.e. $C_{10}H_{20}O$ (e.g. menthol), $C_{10}H_{18}O$ (e.g. linalool), $C_9H_{12}O_2$ (e.g. phenoxy propanol) and $C_{12}H_{20}O_2$ (e.g. geranyl acetate). Correlations with $C_{10}H_{30}O_5Si_5$ (e.g. D5 siloxane) were also around 0.9. Most of these compounds (except D5) can be found in cleaning products, which likely contributed to $C_{10}H_{18}O$ ion signal since it strongly varied with the same ions but also with $C_{11}H_{22}O_2$ and $C_{19}H_{18}O_2$ (e.g. FAMEs) and $C_{10}H_{20}O_2$ (e.g. hydroxycitronellal).

On the contrary, no ions correlated very strongly (r > 0.95) with D5 siloxane but 13 ions showed r > 0.9. Menthol- and linalool-containing ions showed the best correlations with D5 (r ~ 0.93) followed by several $C_xH_yO_2$ ions such as $C_{12}H_{20}O_2$ (e.g. α-terpinyl acetate) and $C_9H_{10}O_2$ (e.g. benzyl acetate), which are used in cosmetics and other fragrance-related products. C_7H_8O (e.g. benzyl alcohol) concentrations varied very similarly to several ions containing oxy-terpenoids, monoterpenes, D5 siloxane and acetates that are found in cosmetic products.

Fragrances and related solvents likely also contributed to $C_7H_{14}O_2$ (e.g. amyl acetate) since it showed very strong correlations with $C_4H_6O_2$, $C_8H_{14}O_2$, C_7H_8O, $C_8H_{16}O$ and $C_{10}H_{20}O$ ions. The highest correlations (r>0.96) were observed with $C_8H_{16}O$ (e.g. octanal) and C_7H_8O (e.g. benzyl alcohol) suggesting that fragrance-based products were likely important contributors of $C_7H_{14}O_2$. Similarly, $C_8H_{16}O_2$ (e.g. caprylic acid) also exhibited similar variations as fragrance-related esters and solvents, and correlated strongly with $C_7H_{14}O_2$ suggesting possible similar sources.

$C_{12}H_{24}O_2$ (e.g. lauric acid) was reasonably correlated (r ~ 0.9) with $C_8H_{14}O_2$, $C_{10}H_{18}O_2$, $C_8H_{16}O_4$ and $C_8H_{16}O$ that are prominently used in fragrances. Among other semivolatile ions, $C_{18}H_{34}O_2$ (e.g. oleic acid), did not show appreciable correlation with other ions potentially due to variations in emissions pathways, sources and gas-to-particle partitioning effects.

Nitrogen-containing species

Among the nitrogen-containing ions measured, C_2H_7NO (e.g. monoethanolamine) correlated strongly with $C_{10}H_{30}O_5Si_5$ (e.g. D5) except the period when it was influenced by biomass burning. C_2H_7NO also correlated very strongly (r > 0.9) with $C_4H_8O_2$ (e.g. ethyl acetate) and with some solvents. Unlike C_2H_7NO, $C_4H_{11}NO_2$ (e.g. diethanolamine) did not show appreciable correlation with tracers of personal care products such as D5 siloxane. This could be due to diethanolamine being primarily used as feedstock for the production of diethanolamides and diethanolamine salts of fatty acids that are used in cosmetic products. Triethanolamine showed very weak correlations (r < 0.85) with majority of the measured ions. Its timeseries varied somewhat similarly with only some aldehyde- and ester-containing ions that are prevalent in fragrance-related products (e.g. phenoxyethyl isobutyrate, pentanal). This suggested that triethanolamine is also likely emitted from personal care products where it sees common usage, though with potential partitioning limitations.

Fatty acid methyl esters

FAME-containing ions strongly correlated with each other suggesting overlap in their sources in urban environments. $C_9H_{18}O_2$ (e.g. methyl octanoate) also correlated strongly with ions containing menthol, octanal, benzyl acetone, hydroxycitronellal and esters that are prevalent in personal care products. Some correlation was also observed with ions containing carbonyl solvents that are used in both consumer and other commercial products suggesting multiple source contributions to $C_9H_{18}O_2$. The same ions formed the best set of correlations for $C_{11}H_{22}O_2$ (e.g. methyl decanoate).

Texanol and TXIB

$C_{12}H_{24}O_3$ (e.g. texanol) which is a tracer for water-based paints. $C_{16}H_{30}O_4$ represents TXIB that is found in a variety of architectural products (Gkatzelis et al., 2021). They did not correlate significantly with each other given some variations in their use. In fact, $C_{12}H_{24}O_3$ correlated considerably ($r > 0.85$) only with the $C_8H_{18}O_2$ ion related to EGHE which is also found in water-based coatings among other wider uses. On the other hand, $C_{16}H_{30}O_4$ showed good correlation with a wider range of compounds and the concentrations of $C_{16}H_{30}O_4$ also exceeded $C_{12}H_{24}O_3$ throughout the measurement period. The strongest similarities in its timeseries were observed with ions containing glycol ethers prevalent in paint-related products, but aromatic esters (e.g. $C_9H_{10}O_2$; benzyl acetate) and some oxy-terpenoids-related ions (e.g. $C_{10}H_{20}O$; menthol, $C_{10}H_{18}O$; linalool) showed good correlation with $C_{16}H_{30}O_4$.

$C_3H_8O_3$ (e.g. glycerol) showed particularly strong correlation with $C_3H_6O_2$ that is related to methyl acetate, propanoic acid and/or ethyl formate. $C_8H_8O_3$ (e.g. methyl paraben) varied similarly as $C_9H_{12}O_2$ (e.g. phenoxy propanol), $C_5H_6O_2$ (e.g. furfuryl alcohol) and C_7H_8O (e.g. benzyl alcohol) that are used in personal care products (except furfuryl alcohol). It also correlated with oxy-terpenoids found in fragrance-related products.

Figure S1. Aerial visualization (© Google Maps) of the sampling location at the ASRC (City University of New York), with view from NNW. The instrument inlet pointed toward downtown Manhattan shown in the distance in the top-right of the image.

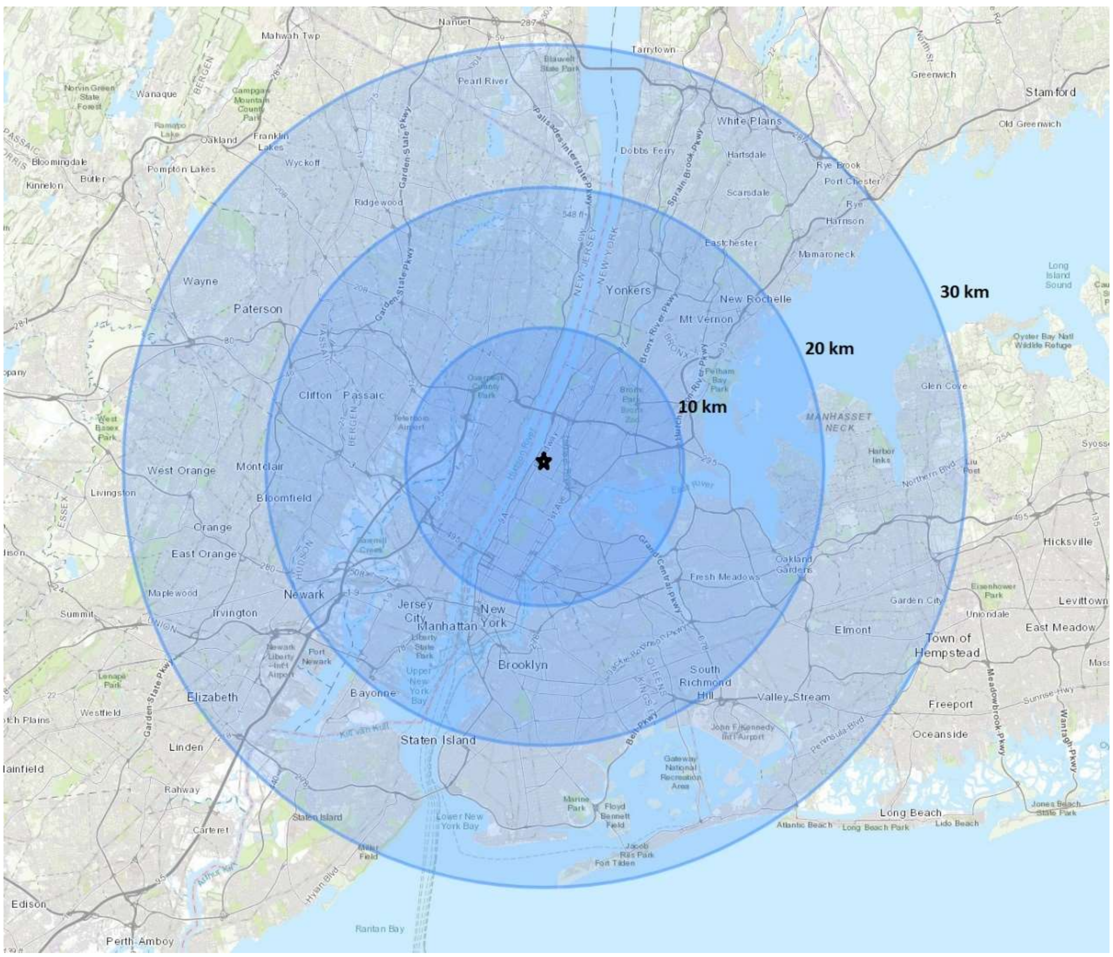

Figure S2. Regional map showing radial distances of 10, 20 and 30 kilometers from the sampling site (starred) at the ASRC (City University of New York). Credits: https://www.calcmaps.com/map-radius/

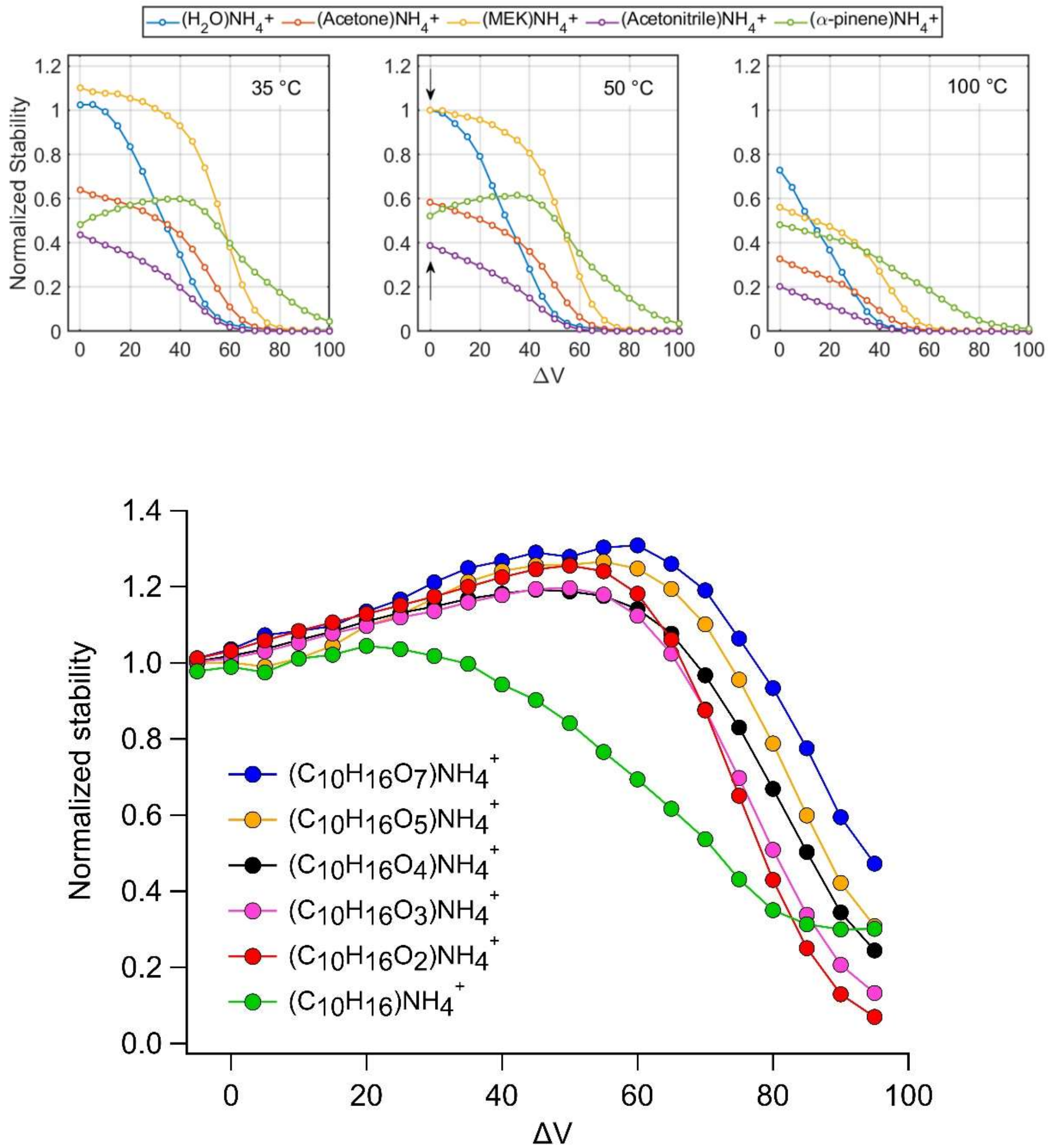

Figure S3. Stability of ammonium-parent ion adducts as a function of voltage and IMR temperature for select compounds including highly oxygenated species.

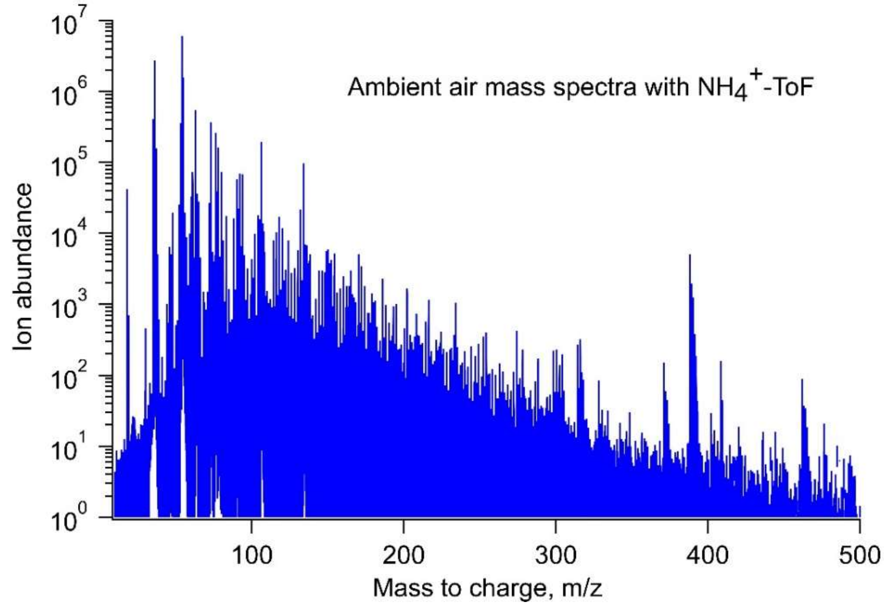

Figure S4. Average ambient air mass spectra collected using Vocus CI-ToF with NH_4^+ as the reagent ion.

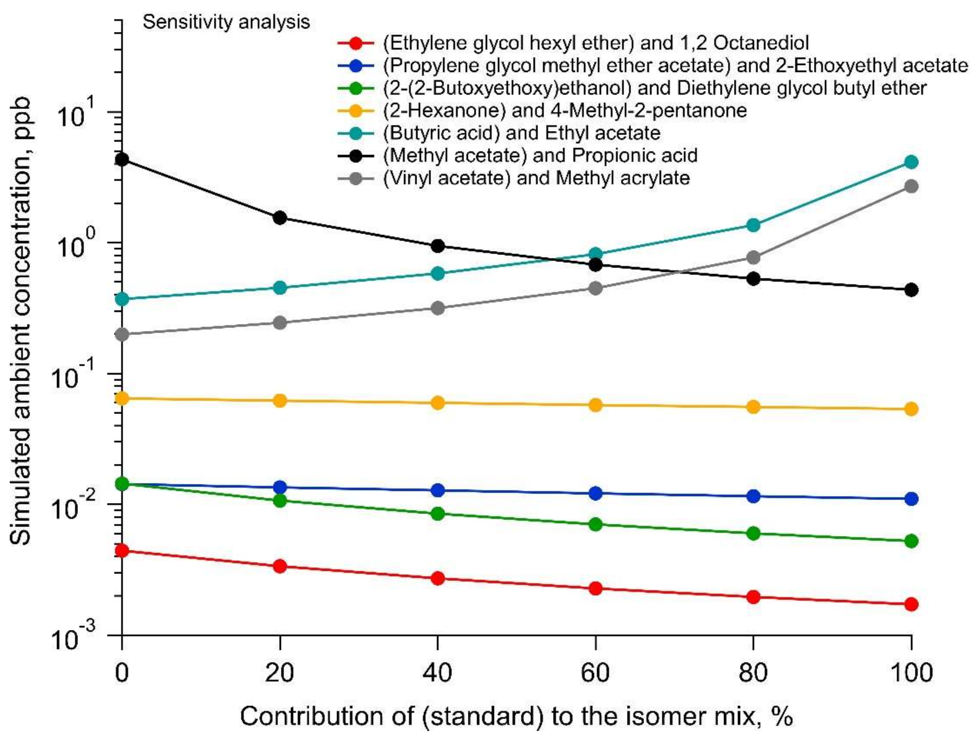

Figure S5. Sensitivity analysis of CI-ToF response factors comparing isomer pairs with variations in instrument sensitivity to NH_4^+ ionization (using calibration standards); shown as variations in simulated concentrations of select ion formulas in response to the changes in the magnitude of the mass calibration factor dependent on relative contribution of each isomer in the pair (x-axis).

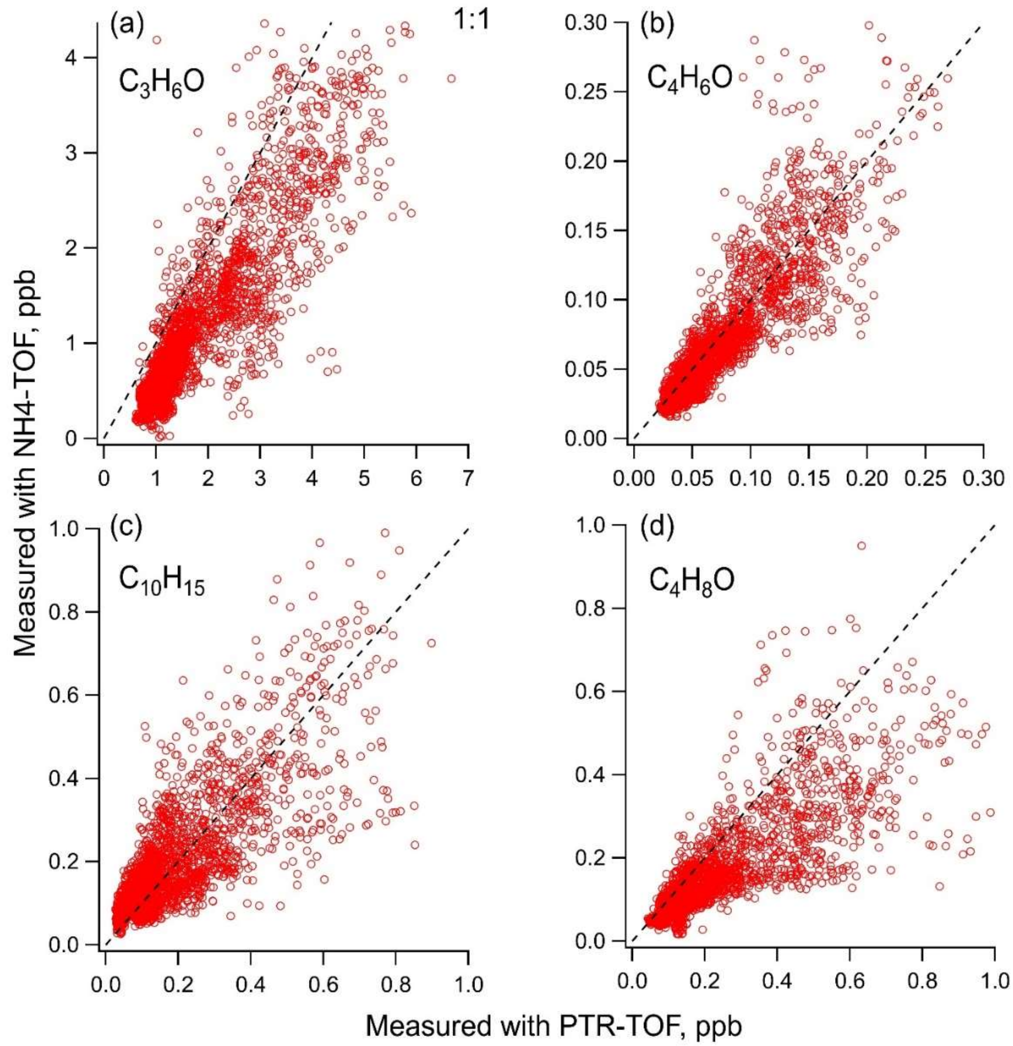

Figure S6. A comparison between measured concentrations of select analytes by NH_4-ToF and co-located PTR-ToF (Stony Brook University) instruments over the sampling period. The spread observed in comparisons of $C_{10}H_{16}$ and C_4H_8O could largely be attributed to variations within relative responses to isomers with the different ionization schemes of the two instruments.

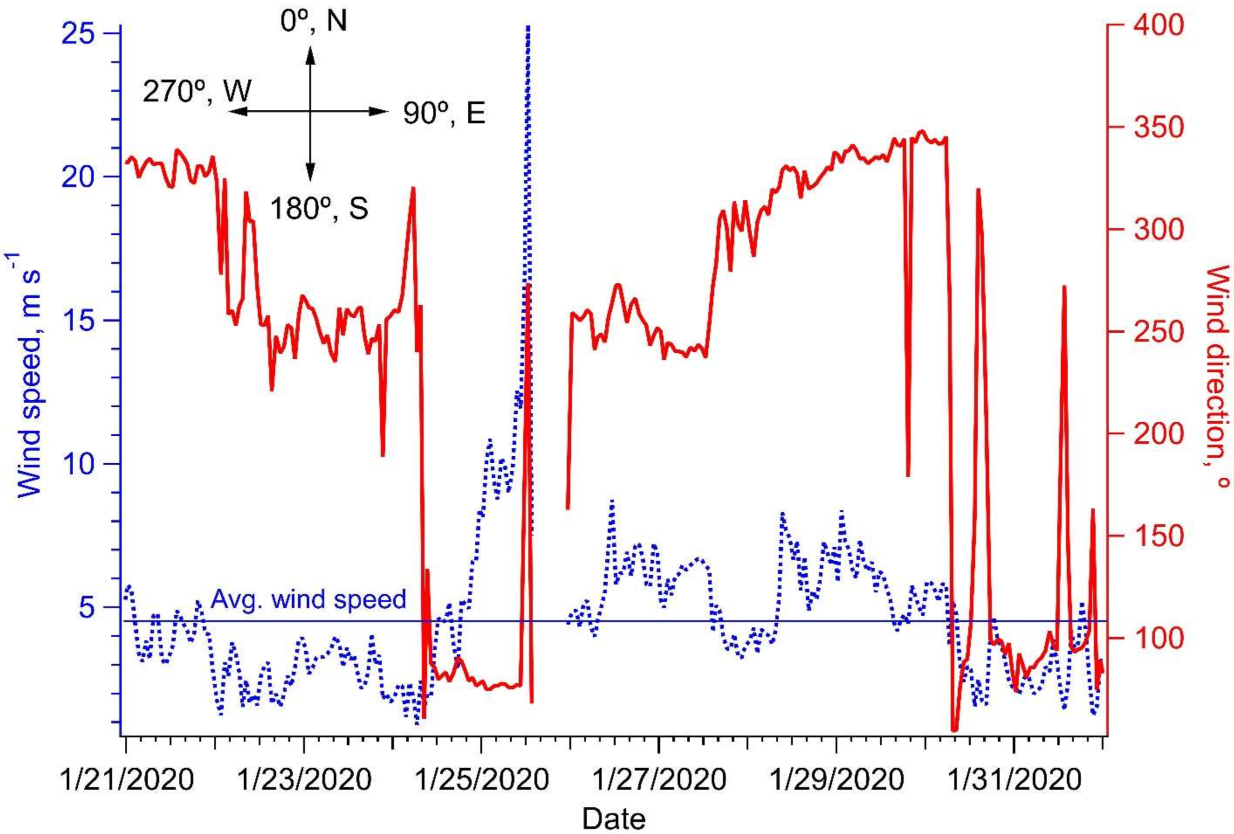

Figure S7. Wind speed and direction at the sampling site during the measurement period. The missing data for the on-site weather station included a period of high wind speeds and periodic heavy rain in the afternoon (until 4:30 LT) followed by calm conditions with winds from South-Northeast between 12-7 PM and West-Northwest thereafter as shown by regional data from the LaGuardia weather station.

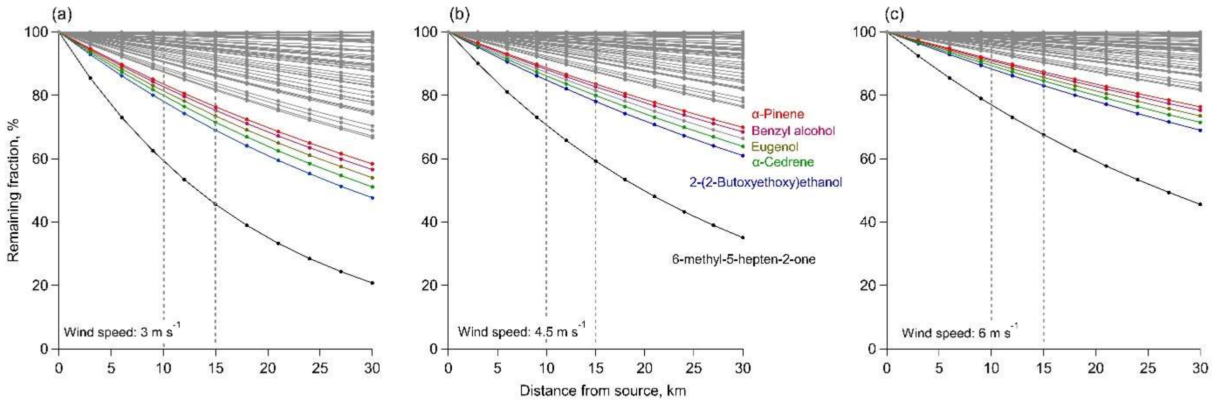

Figure S8. Potential chemical losses due to OH oxidation, shown as fraction remaining with distance after wintertime daytime atmospheric oxidation at different wind speeds for the chemical species listed in table S2. Note: An aerial distance of 10-15 kilometers from the sampling site at ASRC, CUNY covers the commercial areas of New York City, as well as, parts of New Jersey as shown in Figure S2. Daytime monoterpene and sesquiterpene losses may vary between specific isomers, but are shown here as α-pinene and α-cedrene, respectively.

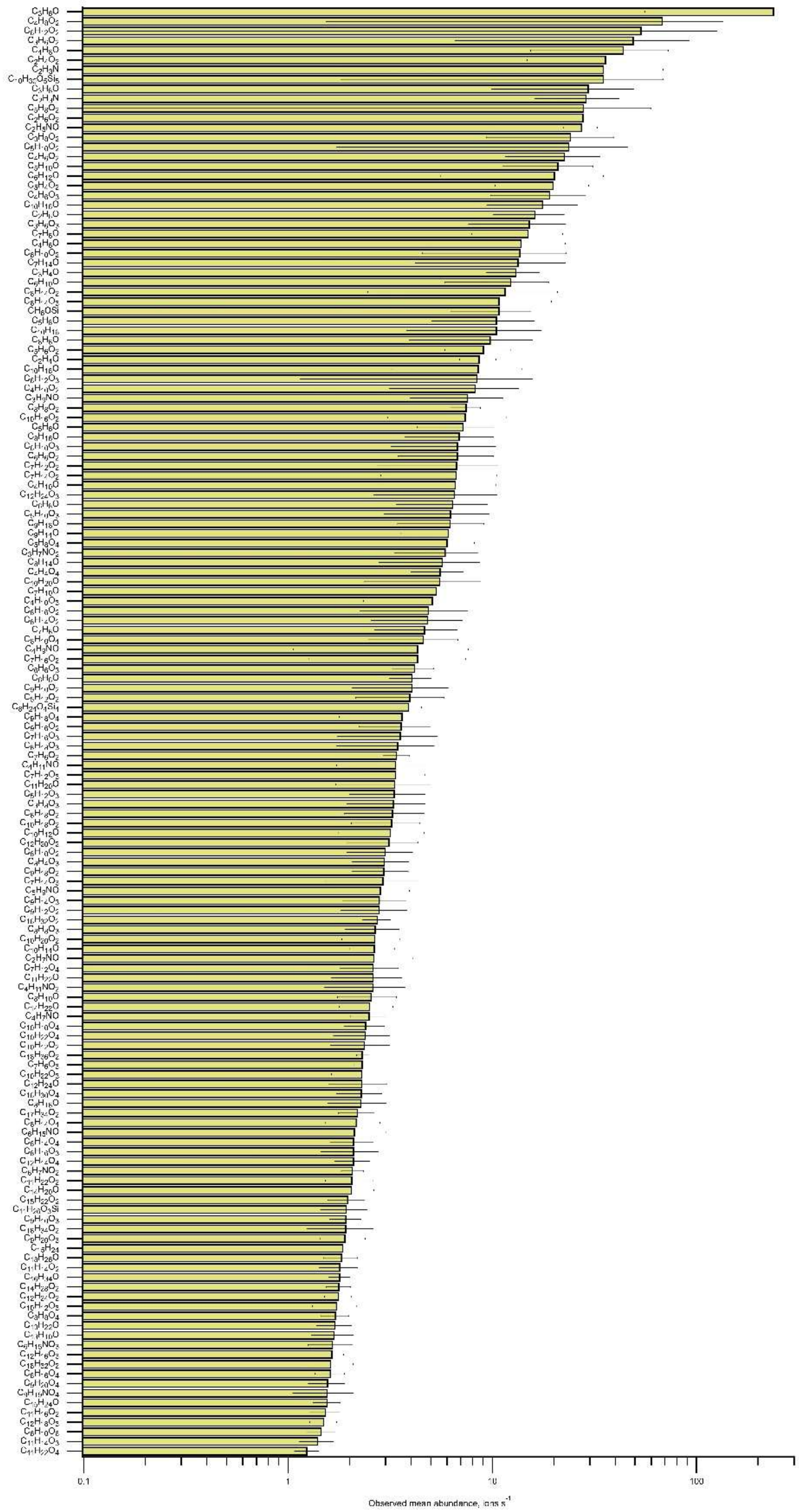

Figure S9. Geometric mean ion abundances of all measured ions averaged over the duration of the sampling campaign.

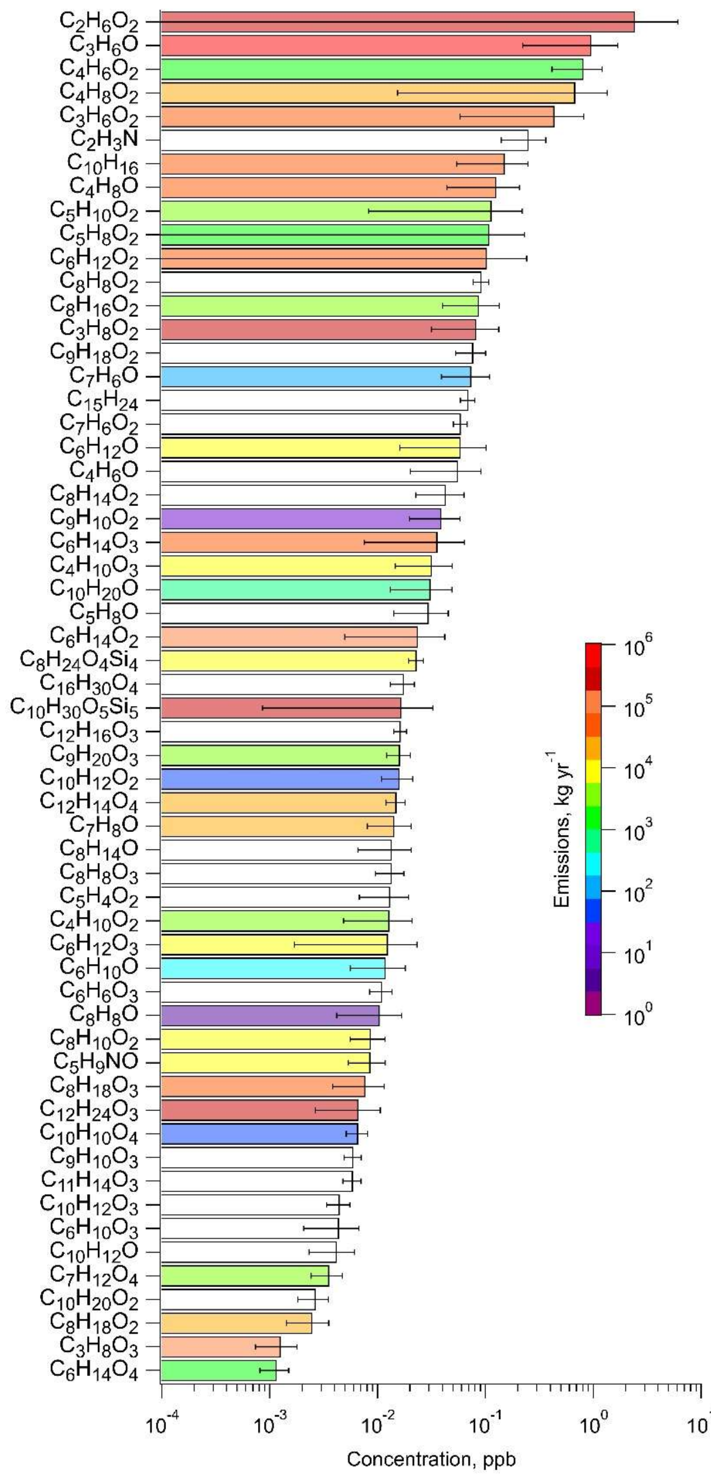

Figure S10. Geometric mean of absolute concentrations (i.e. without 5[th] percentile background subtraction) of mass calibrated ions averaged over the entire duration of the sampling campaign and color coded by their annual emissions as estimated by the VCPy inventory.

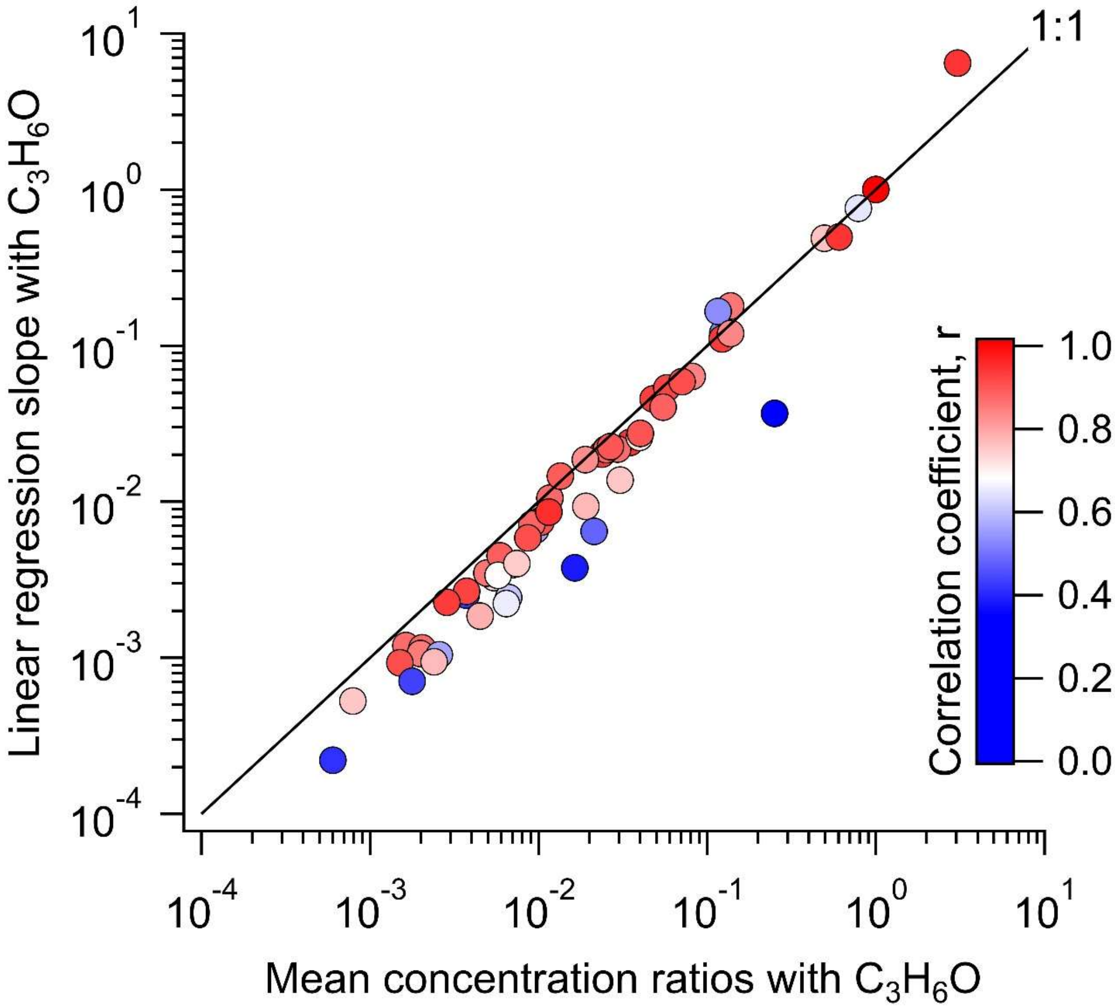

Figure S11. Concentration ratios of measured analytes relative to acetone as determined by linear regression slopes (y-axis) compared to background-subtracted geometric mean concentration ratios (x-axis) and colored by correlation coefficient.

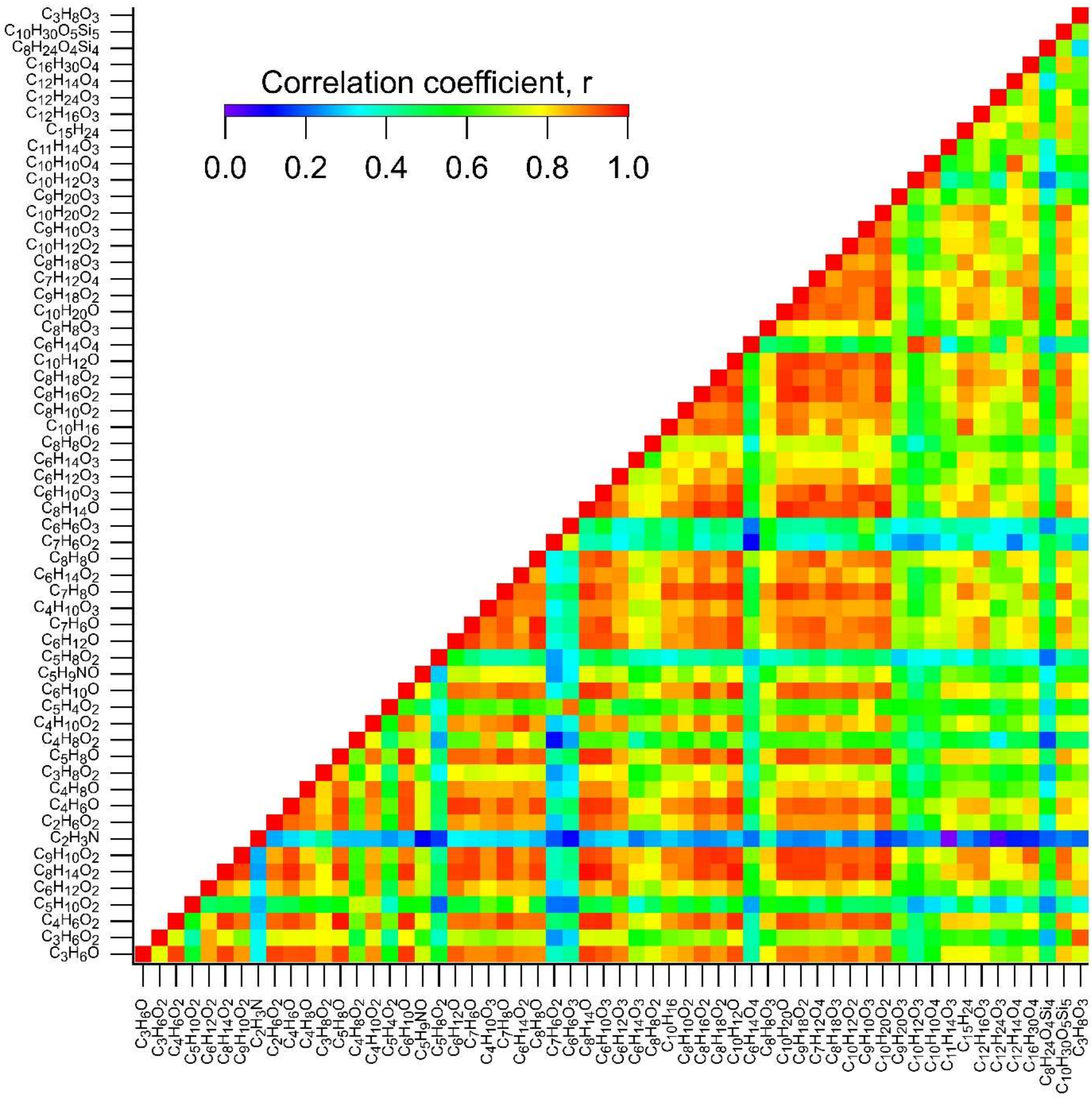

Figure S12. Image-based representation of the various degrees of concentration-based linear correlations between mass calibrated compound pairs.

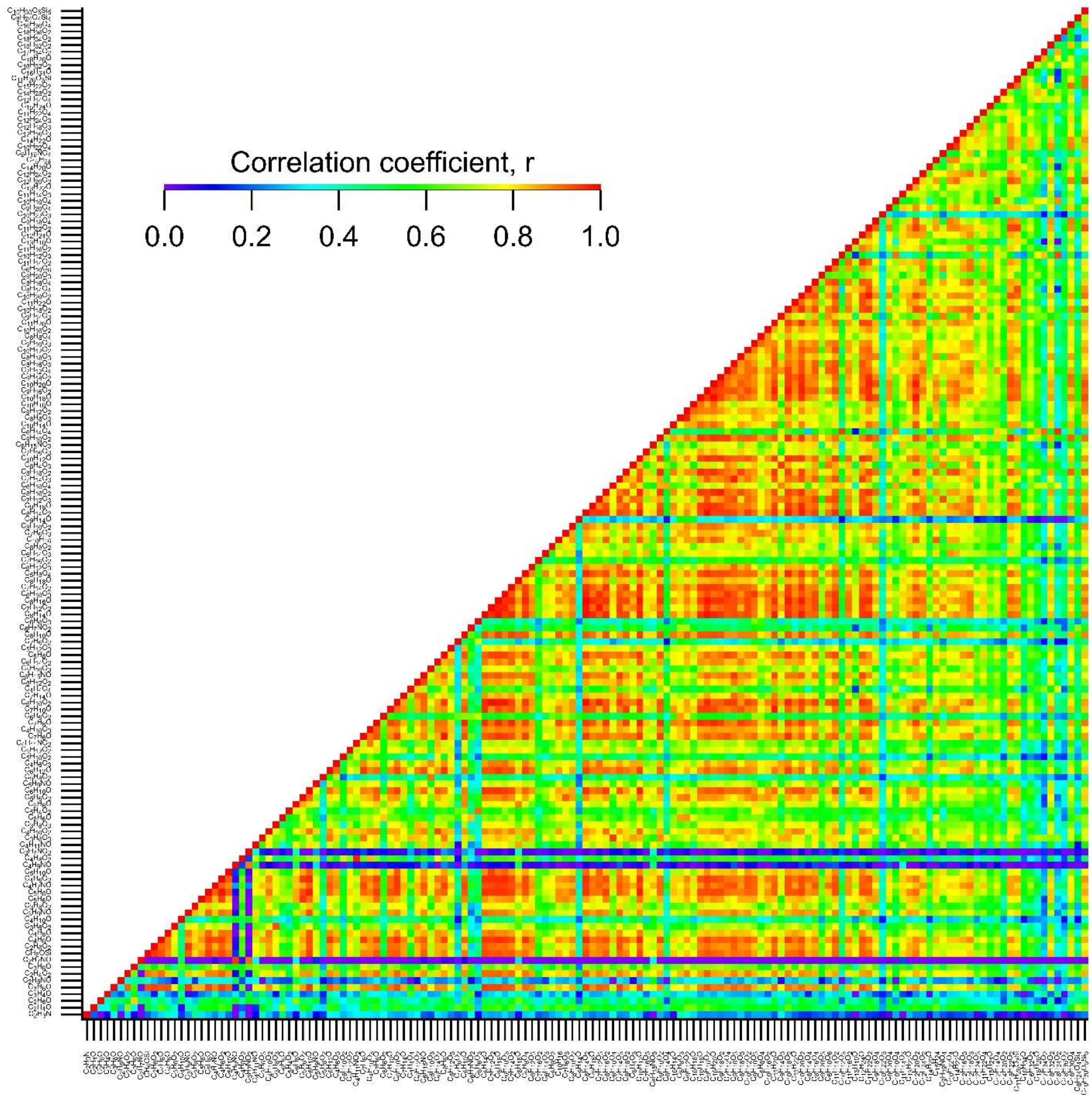

Figure S13. Image-based representation of the various degrees of ion abundance-based linear correlations between all measured ions.

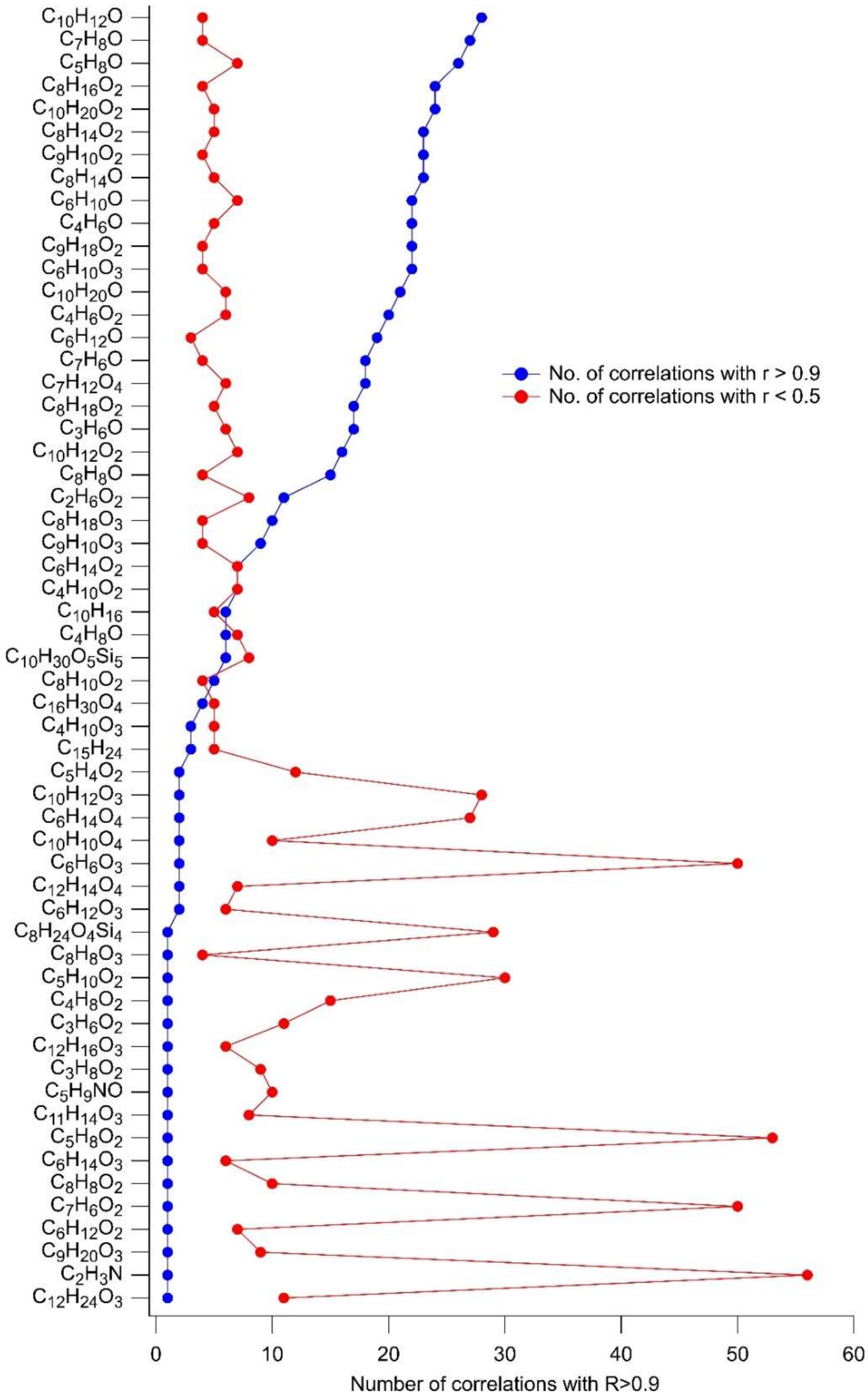

Figure S14. List of measured formulas sorted by ions with the highest counts of concentration-based large correlation coefficients exceeding 0.9. The number of poor correlations (i.e. < 0.5) for each compound is also shown.

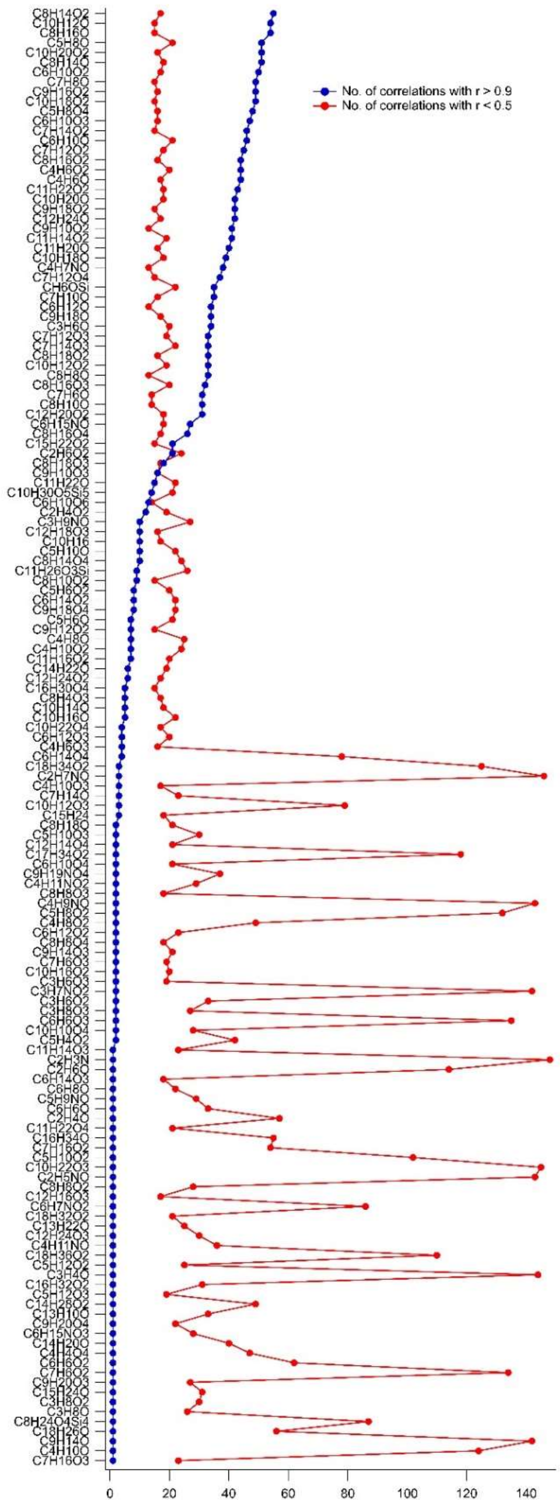

Figure S15. The complete list of targeted ion formulas sorted by ions with the highest counts of ion abundance-based correlation coefficients exceeding 0.9. The number of poor correlations (i.e. < 0.5) for each compound is also shown.

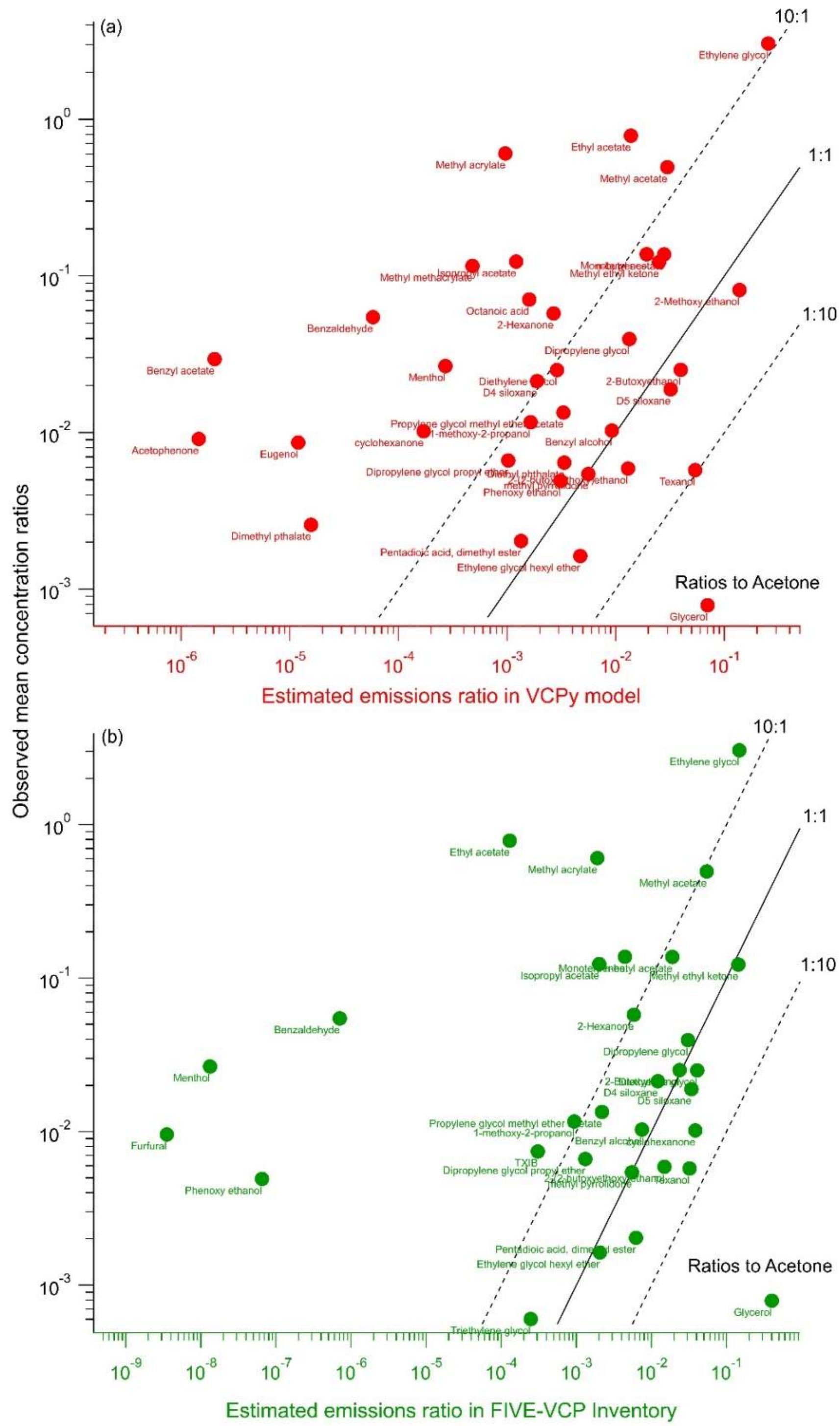

Figure S16. Concentration ratios versus annual emissions inventories (compared to acetone), labelled as likely isomers. Note: Supporting figure for Figure 4 showing same data.

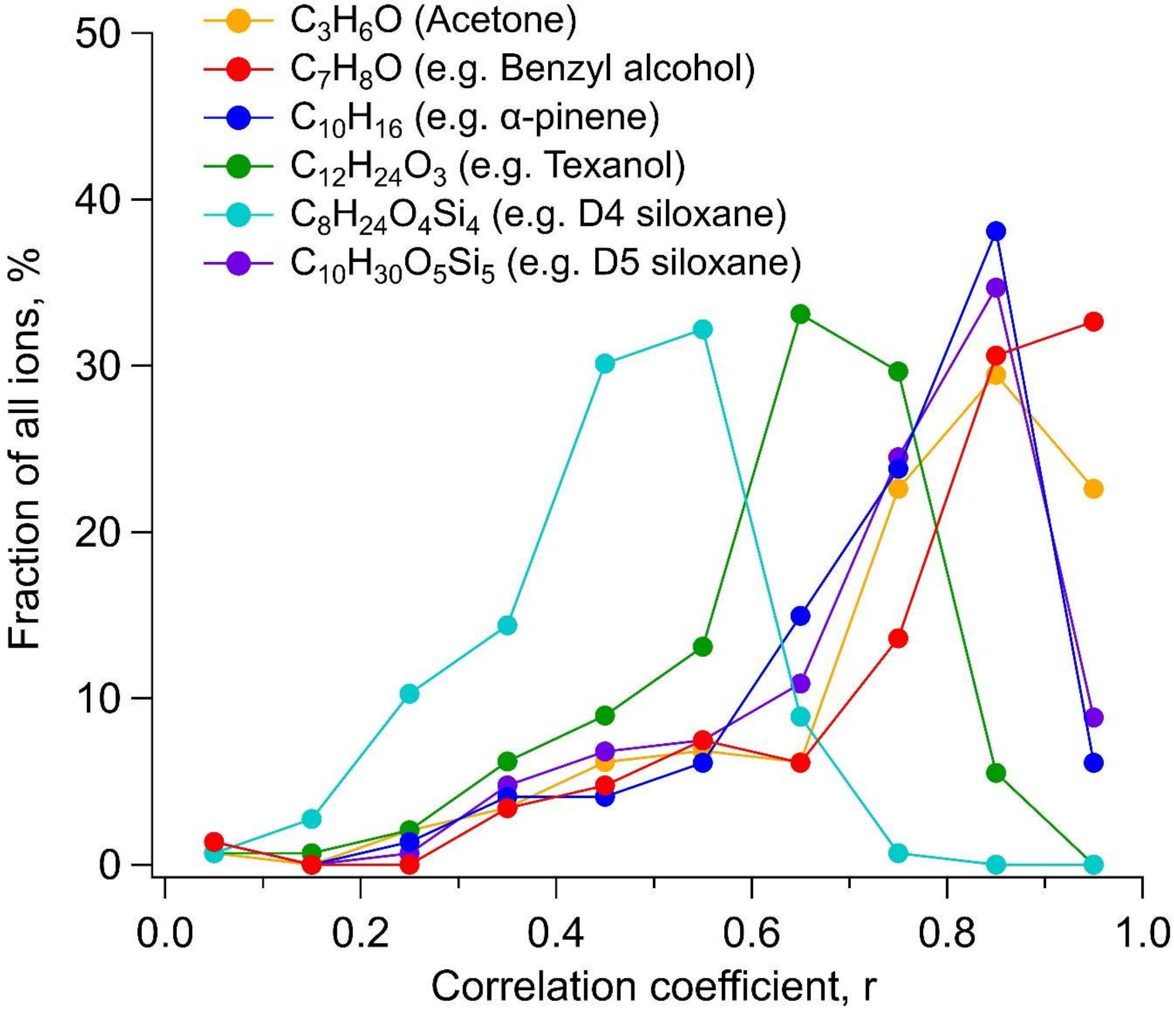

Figure S17. Comparison of correlation coefficients against select tracer compounds using ion abundances of all target species. Nearly 35% of the measured ions correlated highly ($0.9 < r < 1$) with benzyl alcohol's ion.

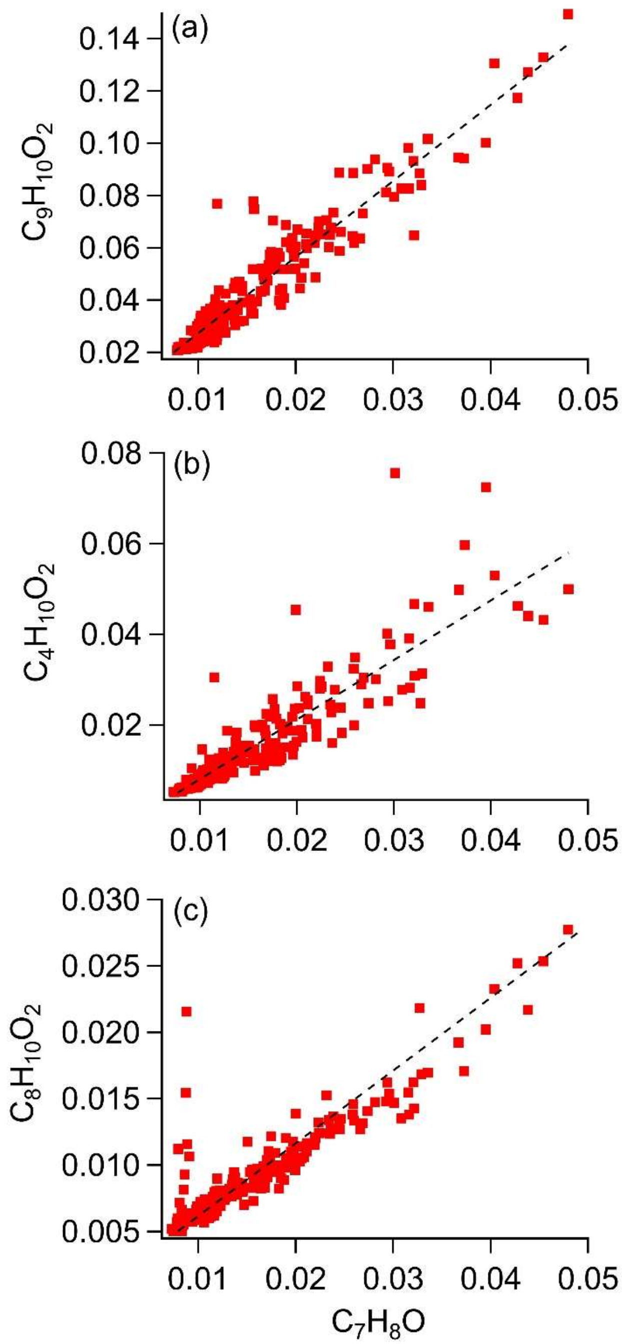

Figure S18. Examples of observed strong linear correlations between C_7H_8O (e.g. benzyl alcohol) and, (a) $C_9H_{10}O_2$ (e.g. benzyl acetate) (b) $C_4H_{10}O_2$ (e.g. 1-methoxy-2-propanol) and (c) $C_8H_{10}O_2$ (e.g. phenoxyethanol)

Table S1. Chemical composition of the analytical standard cylinder (Apel-Riemer Environmental) used for mass calibration of select species.

Multicomponent calibration mixture in nitrogen	
Compound	Concentration (ppb), (uncertainty: 5%)
Ethanol	981
Acetonitrile	993
Acetone	989
Acrylonitrile	987
Isoprene	954
Methyl vinyl ketone	997
Methyl ethyl ketone	994
Benzene	989
o-Xylene	1003
a-Pinene	1000
1,2,4-Trimethylbenzene	973
Octamethylcyclotetrasiloxane	968
Decamethylcyclopentasiloxane	962
b-Caryophyllene	99.5

Table S2. Mass response factors (and standard deviations) for mass calibration of select measured ions (using analytical standards; e.g. AccuStandard, Sigma-Aldrich). Standard deviations are determined based on linear regressions with multi-point LCS calibration curves. Cylinder-based standard calibrations are shown in italics (i.e. Table S1).

Analytical standard	Formula	Res. fac. (avg)	Res. fac. (st. dev)
Glycerol	$C_3H_8O_3$	2617	923
D5-siloxane	$C_{10}H_{30}O_5Si_5$	2200	110
Triethylene glycol	$C_6H_{14}O_4$	1876.504	71
Ethyl acetoacetate	$C_6H_{10}O_3$	1548.422	112
Furfural	$C_5H_4O_2$	1522	64
Ethylene glycol hexyl ether	$C_8H_{18}O_2$	1320.445	40
Cyclohexanone	$C_6H_{10}O$	1042.756	69
Hydroxycitronellal	$C_{10}H_{20}O_2$	1007.586	63
Texanol	$C_{12}H_{24}O_3$	995.1243	65
Acetophenone	C_8H_8O	937.9794	20
Benzyl acetone	$C_{10}H_{12}O$	761.2294	86
Pentadioic acid, dimethyl ester	$C_7H_{12}O_4$	737.1291	60
Propylene glycol methyl ether acetate	$C_6H_{12}O_3$	679.011	55
1-Methoxy-2-propanol	$C_4H_{10}O_2$	645.9141	69
n-Butyl acetate	$C_6H_{12}O_2$	521.7066	34
2-Butoxyethanol	$C_6H_{14}O_2$	495.2152	40
2-(2-Butoxyethoxy)ethanol	$C_8H_{18}O_3$	450.3138	184
6-Methyl 5-hepten-2-one	$C_8H_{14}O$	424.3785	11
Propyl paraben	$C_{10}H_{12}O_3$	389.7354	74
Maltol	$C_6H_6O_3$	380.425	37
Dimethyl phthalate	$C_{10}H_{10}O_4$	366.3753	23
Cyclopentanone	C_5H_8O	355.6696	9
Methyl ethyl ketone	C_4H_8O	350	18
2-Hexanone	$C_6H_{12}O$	345.8968	18
Phenoxy ethanol	$C_8H_{10}O_2$	345.677	119
Methyl pyrrolidone	C_5H_9NO	331.8216	41
Benzyl alcohol	C_7H_8O	329.976	23
Ethyl paraben	$C_9H_{10}O_3$	323.4804	73
Dipropylene glycol	$C_6H_{14}O_3$	303.4106	43
2-Methoxy ethanol	$C_3H_8O_2$	295.6414	30
Methyl methacrylate	$C_5H_8O_2$	260	13
Acetone	C_3H_6O	251	13
MVK	C_4H_6O	250	12
Butyl paraben	$C_{11}H_{14}O_3$	238.0273	43
Isopropyl acetate	$C_5H_{10}O_2$	209.0689	23
Benzaldehyde	C_7H_6O	203.1	14
Methyl paraben	$C_8H_8O_3$	199.2943	53
Menthol	$C_{10}H_{20}O$	180.1444	11
D4-siloxane	$C_8H_{24}O_4Si_4$	170.36	52.26
Diethylene glycol	$C_4H_{10}O_3$	160.6576	28
Eugenol	$C_{10}H_{12}O_2$	148.3496	7
Diethyl phthalate	$C_{12}H_{14}O_4$	140.7306	8
TXIB	$C_{16}H_{30}O_4$	131.0738	14
Dipropylene glycol propyl ether	$C_9H_{20}O_3$	118.3448	15
Acetonitrile	C_2H_3N	115	6
Methyl acetate	$C_3H_6O_2$	113.0	6
Cyclohexyl acetate	$C_8H_{14}O_2$	112.9	6
Benzyl acetate	$C_9H_{10}O_2$	104.4707	10
2-Phenoxyethyl isobutyrate	$C_{12}H_{16}O_3$	100.8308	9
Butyric acid	$C_4H_8O_2$	100.464	19
Methyl benzoate	$C_8H_8O_2$	81.46912	6
Monoterpenes	$C_{10}H_{16}$	70	3
Benzoic acid	$C_7H_6O_2$	57.82037	4
Octanoic acid	$C_8H_{16}O_2$	56.12189	4
Methyl octanoate	$C_9H_{18}O_2$	38.58139	3
Vinyl acetate	$C_4H_6O_2$	28	2
Sesquiterpenes	$C_{15}H_{24}$	27	1
Ethylene glycol	$C_2H_6O_2$	11.48517	1

Table S3. Geometric mean ion abundances (ions s^{-1}) and standard deviations measured for all calibrated and non-calibrated ions.

Ion formula	Mean abundance ± standard deviation	Ion formula	Mean abundance ± standard deviation	Ion formula	Mean abundance ± standard deviation
C_3H_6O	239.76±183.96	C_6H_8O	6.46±3.06	$C_4H_{11}NO_2$	2.62±1.11
$C_4H_8O_2$	68.26±66.72	$C_5H_{10}O_3$	6.29±3.34	$C_8H_{10}O$	2.57±0.82
$C_6H_{12}O_2$	53.77±71.95	$C_9H_{18}O$	6.25±2.82	$C_{14}H_{22}O$	2.52±0.74
$C_3H_6O_2$	49.2±42.65	$C_9H_{14}O$	6.13±2.57	C_4H_7NO	2.51±0.49
C_4H_8O	43.98±28.61	$C_5H_8O_4$	6.05±2.1	$C_{10}H_{10}O_4$	2.42±0.54
$C_2H_4O_2$	36.06±21.25	$C_3H_7NO_2$	5.92±2.61	$C_{10}H_{22}O_4$	2.4±0.74
$C_{10}H_{30}O_5Si_5$	35.12±33.31	$C_8H_{14}O$	5.74±2.96	$C_{10}H_{12}O_2$	2.38±0.76
C_3H_8O	29.66±19.76	$C_4H_4O_4$	5.59±1.59	$C_{18}H_{36}O_2$	2.33±0.16
C_2H_3N	28.91±12.8	$C_{10}H_{20}O$	5.57±3.22	$C_7H_6O_3$	2.32±0.22
$C_5H_8O_2$	28.07±31.59	$C_7H_{10}O$	5.35±3.01	$C_{10}H_{22}O_3$	2.31±0.69
$C_2H_6O_2$	27.99±41.6	$C_4H_{10}O_3$	5.11±2.77	$C_{12}H_{24}O$	2.31±0.73
C_2H_5NO	27.5±5.14	$C_8H_{16}O_2$	4.89±2.65	$C_{16}H_{30}O_4$	2.3±0.57
$C_3H_8O_2$	24.32±14.97	$C_8H_{14}O_2$	4.85±2.3	$C_8H_{18}O$	2.29±0.73
$C_5H_{10}O_2$	23.79±22.06	C_7H_8O	4.7±2.05	$C_{17}H_{34}O_2$	2.2±0.44
$C_4H_6O_2$	22.68±11.09	$C_6H_{10}O_4$	4.62±2.15	$C_6H_{14}O_4$	2.17±0.65
$C_5H_{10}O$	21.12±9.91	C_4H_9NO	4.35±3.29	$C_6H_{15}NO$	2.12±0.9
$C_6H_{12}O$	20.24±14.68	$C_7H_{16}O_2$	4.34±3.08	$C_8H_{14}O_4$	2.11±0.51
$C_5H_4O_2$	19.93±9.62	$C_6H_6O_3$	4.18±0.97	$C_8H_{16}O_3$	2.11±0.66
$C_4H_6O_3$	19.25±9.42	C_6H_6O	4.07±0.94	$C_{12}H_{14}O_4$	2.11±0.42
$C_{10}H_{16}O$	17.72±8.34	$C_9H_{10}O_2$	4.07±2.01	$C_6H_7NO_2$	2.08±0.26
C_2H_6O	16.29±6.17	$C_5H_{12}O_2$	3.97±1.83	$C_{11}H_{22}O_2$	2.07±0.55
$C_3H_6O_3$	15.28±7.64	$C_8H_{24}O_4Si_4$	3.91±0.6	$C_{14}H_{20}O$	2.05±0.58
C_7H_6O	15.03±7.09	$C_9H_{18}O_4$	3.64±1.86	$C_{15}H_{22}O_2$	1.97±0.4
C_4H_6O	13.89±8.85	$C_9H_{16}O_2$	3.61±1.38	$C_{11}H_{26}O_3Si$	1.94±0.5
$C_6H_{10}O_2$	13.75±9.21	$C_7H_{16}O_3$	3.57±1.82	$C_9H_{10}O_3$	1.93±0.34
$C_7H_{14}O$	13.47±9.28	$C_8H_{18}O_3$	3.46±1.73	$C_{18}H_{34}O_2$	1.93±0.69
C_3H_4O	13.13±3.82	$C_7H_6O_2$	3.42±0.5	$C_9H_{20}O_3$	1.91±0.47
$C_6H_{10}O$	12.39±6.54	$C_4H_{11}NO$	3.38±1.66	$C_{15}H_{24}$	1.87±0.29
$C_6H_{14}O_2$	11.62±9.17	$C_7H_{12}O_3$	3.38±1.29	$C_{18}H_{26}O$	1.84±0.34
$C_6H_{14}O_3$	10.87±8.58	$C_{11}H_{20}O$	3.35±1.64	$C_{11}H_{14}O_2$	1.81±0.38
CH_6OSi	10.85±4.6	$C_5H_{12}O_3$	3.34±1.34	$C_{16}H_{34}O$	1.8±0.21
C_5H_8O	10.56±5.52	$C_3H_8O_3$	3.31±1.37	$C_{14}H_{28}O_2$	1.78±0.24
$C_{10}H_{16}$	10.55±6.75	$C_8H_{18}O_2$	3.27±1.39	$C_{12}H_{24}O_2$	1.78±0.27
C_8H_8O	9.82±5.9	$C_{10}H_{18}O_2$	3.23±1.19	$C_{10}H_{12}O_3$	1.74±0.42
$C_5H_6O_2$	9.1±3.23	$C_{10}H_{12}O$	3.19±1.43	$C_8H_8O_4$	1.72±0.27
C_2H_4O	8.67±1.77	$C_{12}H_{20}O_2$	3.14±1.19	$C_{13}H_{22}O$	1.71±0.33
$C_{10}H_{18}O$	8.58±5.34	$C_8H_{10}O_2$	3±1.07	$C_{13}H_{10}O$	1.69±0.39
$C_6H_{12}O_3$	8.45±7.3	$C_8H_4O_3$	2.98±0.92	$C_6H_{15}NO_3$	1.66±0.41
$C_4H_{10}O_2$	8.29±5.17	$C_9H_{18}O_2$	2.96±0.91	$C_{12}H_{16}O_3$	1.65±0.22
C_3H_9NO	7.62±3.67	$C_7H_{14}O_3$	2.94±1.41	$C_{18}H_{32}O_2$	1.62±0.46
$C_8H_8O_2$	7.49±1.25	C_5H_9NO	2.85±1.07	$C_8H_{16}O_4$	1.62±0.27
$C_{10}H_{16}O_2$	7.41±4.34	$C_9H_{14}O_3$	2.82±0.97	$C_9H_{20}O_4$	1.58±0.32
C_5H_6O	7.22±2.94	$C_9H_{12}O_2$	2.81±1	$C_9H_{19}NO_4$	1.57±0.51
$C_8H_{16}O$	6.92±3.2	$C_{16}H_{32}O_2$	2.75±0.43	$C_{15}H_{24}O$	1.56±0.24
$C_6H_{10}O_3$	6.8±3.59	$C_8H_8O_3$	2.69±0.8	$C_{11}H_{16}O_2$	1.53±0.26
$C_6H_6O_2$	6.79±3.34	$C_{10}H_{20}O_2$	2.68±0.84	$C_{12}H_{18}O_3$	1.5±0.23
$C_7H_{12}O_2$	6.71±3.96	$C_{10}H_{14}O$	2.66±0.65	$C_6H_{10}O_6$	1.46±0.23
$C_7H_{14}O_2$	6.69±3.85	C_2H_7NO	2.65±1.42	$C_{11}H_{14}O_3$	1.4±0.27
$C_4H_{10}O$	6.63±3.77	$C_7H_{12}O_4$	2.62±0.84	$C_{11}H_{22}O_4$	1.25±0.17
$C_{12}H_{24}O_3$	6.58±3.95	$C_{11}H_{22}O$	2.62±0.99		

Table S4. List of the calibrated ion formulas measured using the NH_4^+-ToF instrument, their possible chemical names and examples of known uses. Listed examples (for calibrated compounds and other potential isomers) are not intended to be comprehensive, but provide examples of common uses that can aid in the interpretation of observations.

Mass calibrated ions	Analytical standards used	Other likely contributing isomers	Example uses/sources of all listed isomers
$C_{10}H_{30}O_5Si_5$	D5-siloxane		Cosmetic products, antiperspirants
$C_6H_{14}O_4$	Triethylene glycol		Automobile fluids, lubricants, solvents
$C_6H_{10}O_3$	Ethyl acetoacetate		
$C_5H_4O_2$	Furfural		Feedstock chemical, specialty solvent, wood off-gassing, biomass burning
$C_8H_{18}O_2$	Ethylene glycol hexyl ether; 1,2 Octanediol		
$C_6H_{10}O$	Cyclohexanone		Solvent for paints, degreasers, polymers, etc.
$C_{10}H_{20}O_2$	Hydroxycitronellal	Octyl acetate, p-Menthane-3,8-diol	Fragrances, solvents, insect repellants
$C_{12}H_{24}O_3$	Texanol		Paint solvent, other solvents
C_8H_8O	Acetophenone	2-methyl benzaldehyde, phenyl acetaldehyde	Automobile exhaust, fragrances
$C_{10}H_{12}O$	Benzyl acetone	Anethole, Estragole, Cuminaldehyde	Perfumery, cosmetic products
$C_7H_{12}O_4$	Pentadioic acid, dimethyl ester	Diethyl malonate	Fragrances
$C_6H_{12}O_3$	PGMEA; 2-Ethoxyethyl acetate		Coatings, printing inks, deicing formulations
$C_4H_{10}O_2$	1-Methoxy-2-propanol	2-Ethoxyethanol, 1,4 Butanediol	Industrial solvent
$C_6H_{12}O_2$	Butyl acetate	Propyl propanoate, Methyl pentanoate, Ethyl butyrate, Diacetone alcohol	Fragrances, paints, solvents
$C_6H_{14}O_2$	2-Butoxyethanol	2-Methyl-2,4-pentanediol	Solvents, cosmetic products, coatings, surfactant stabilizer
$C_3H_8O_2$	2-Methoxy ethanol; Propylene glycol	Dimethoxymethane	Solvent for varnishes, dyes, wood stains
$C_8H_{18}O_3$	2-(2-Butoxyethoxy)ethanol; DGBE		Paints, inks, surface cleaners, varnishes
$C_8H_{14}O$	6-Methyl 5-hepten-2-one	Filbertone	Skin oil oxidation product, fragrances
$C_{10}H_{12}O_3$	Propyl paraben		Cosmetics
$C_6H_6O_3$	Maltol	Pyrolgallol, Hydroxymethylfurfural	Dyes, other industrial processing, food additive
$C_{10}H_{10}O_4$	Dimethyl pthalate		Insect repellents, lacquer coatings, plastics
C_5H_8O	Cyclopentanone	3-Penten-2-one	Precursor to fragrances, flavoring agent
C_4H_8O	Methyl ethyl ketone	Tetrahydrofuran	Paints, dyes, adhesive remover, degreasers, solvent
$C_6H_{12}O$	2-Hexanone; 4-Methyl-2-pentanone	Methyl isobutyl ketone	Solvent
$C_8H_{10}O_2$	Phenoxy ethanol	Anisyl alcohol, 1,4-Dimethoxybenzene	Fragrances, soaps
C_5H_9NO	Methyl pyrrolidone		Industrial solvent
C_7H_8O	Benzyl alcohol	Anisole	General solvent
$C_9H_{10}O_3$	Ethyl paraben	Ethyl salicylate	Cosmetics
$C_6H_{14}O_3$	Dipropylene glycol	2-(2-Ethoxyethoxy)ethanol	Industrial solvent, paints, wood stains, textile inks, brake fluids
$C_5H_8O_2$	Methyl methacrylate	Acetylpropionyl, 2-Methyltetrahydrofuran-3-one	Solvents for paints, inks and lacquers, coffee aroma
C_3H_6O	Acetone	Propionaldehyde	Wide-use solvent, disinfectant
C_4H_6O	Methyl vinyl ketone	Methacrolein, Crotonaldehyde	Chemical precursor
$C_{11}H_{14}O_3$	Butyl paraben		Antioxidant, cosmetic preservatives
$C_5H_{10}O_2$	Isopropyl acetate; n-Propyl acetate	Isobutyl formate, Methyl isobutyrate	Fragrances, industrial solvent

C_7H_6O	Benzaldehyde		Soaps, dyes, fragrances
$C_8H_8O_3$	Methyl paraben		Cosmetics, personal care products
$C_{10}H_{20}O$	Menthol	Citronellal, Decanal, Rhodinol	Fragrances, insect repellants, food flavoring
$C_4H_{10}O_3$	Diethylene glycol		Solvent for resins, dyes, oils
$C_{10}H_{12}O_2$	Eugenol	Chavibetol, Propyl benzoate, Hinokitiol	Fragrances, cosmetic preservatives, food flavoring, consumer products
$C_{12}H_{14}O_4$	Diethyl phthalate		Plasticizer in consumer products
$C_{16}H_{30}O_4$	TXIB		Inks, coatings, lacquers
$C_9H_{20}O_3$	Dipropylene glycol propyl ether		Industrial solvent, inks, coatings
C_2H_3N	Acetonitrile		Industrial solvent, chemical precursor, combustion by-product
$C_3H_6O_2$	Methyl acetate; Propionic acid	Hydroxyacetone, Ethyl formate	Industrial solvent, naturally occurring
$C_8H_{14}O_2$	Cyclohexyl acetate		Flavoring agent, fragrances
$C_9H_{10}O_2$	Benzyl acetate	Ethyl benzoate, Acetanisole	Fragrances, food flavoring
$C_{12}H_{16}O_3$	2-Phenoxyethyl isobutyrate		
$C_4H_8O_2$	Butyric acid; Ethyl acetate	Methyl propionate, Acetoin	Industrial solvent, coatings, fragrances, food flavoring
$C_8H_8O_2$	Methyl benzoate	Phenylacetic acid	Fragrances
$C_{10}H_{16}$	Monoterpenes		Widely-used fragrances, Food flavoring, biogenic sources
$C_7H_6O_2$	Benzoic acid		Fragrances, dyes, insect repellents
$C_8H_{16}O_2$	Octanoic acid	Hexyl acetate	Disinfectants, skin products, industrial solvent
$C_8H_{24}O_4Si_4$	D4-siloxane		Adhesives, silicone rubbers, gels
$C_9H_{18}O_2$	Methyl octanoate	Heptyl acetate, Pentyl butyrate	Fragrances, cigarette additive
$C_{15}H_{24}$	Sesquiterpenes		Fragrances, biogenic sources
$C_2H_6O_2$	Ethylene glycol	Methoxymethanol	Antifreeze, coolant, de-icing agent, paints, printing inks
$C_4H_6O_2$	Vinyl acetate; Methyl acrylate	γ-Butyrolactone, Methacrylic acid, Diacetyl	Monomer, precursor/feedstock, nail primers, fragrances
$C_3H_8O_3$	Glycerol		Personal care products, foods

Table S5. List of ions calibrated with authentic standards (Table S2), probable contributing isomers, background subtracted geometric mean concentrations (with standard deviations), annual emissions in each inventory, and measured mean concentration ratios (with standard deviations over the measurement period and linear correlation coefficients) with acetone and other prominent combustion-related tracers.

Compound formula, i	Probable compounds, i	Geo. mean concentration, ppt, i	Emissions, kg yr^{-1} VCPy, FIVE-VCP	Ratios to tracer compounds (mol/mol) †			
				Δi/ΔBenzene (r)	Δi*1000/ΔCO (r)	Δi/ΔAcetone (r)	Δi/ΔBenzyl alcohol (r)
$C_2H_6O_2$	Ethylene glycol	2437±3622	361511, 260540	1.1E+01±2.5E+01 (0.79)	9.1E+00±2.0E+01 (0.83)	2.8E+00±6.4E+00 (0.95)	3.0E+02±6.5E+02 (0.88)
C_3H_6O	Acetone*	977±783	1333642, 1647548	3.8E+00±6.7E+00 (0.83)	3.3E+00±5.2E+00 (0.87)	--	1.1E+02±1.6E+02 (0.92)
$C_4H_6O_2$	Methyl acrylate*, Diacetyl*	810±396	1905, 4638	2.1E+00±3.6E+00 (0.82)	1.8E+00±2.7E+00 (0.89)	5.6E-01±8.9E-01 (0.95)	5.9E+01±8.6E+01 (0.94)
$C_4H_8O_2$	Ethyl acetate*, Butyric acid	679±664	27958, 323	2.8E+00±5.3E+00 (0.72)	2.3E+00±4.1E+00 (0.73)	7.2E-01±1.3E+00 (0.73)	7.6E+01±1.3E+02 (0.67)
$C_3H_6O_2$	Methyl acetate*, Propionic acid, Hydroxyacetone, Ethyl formate	435±377	50747, 114453	1.7E+00±3.1E+00 (0.64)	1.5E+00±2.4E+00 (0.65)	4.5E-01±7.9E-01 (0.76)	4.8E+01±7.7E+01 (0.7)
C_2H_3N	Acetonitrile	246±102		8.5E-01±1.2E+00 (0.32)	7.2E-01±9.1E-01 (0.24)	2.2E-01±3.0E-01 (0.35)	2.3E+01±2.8E+01 (0.33)
$C_{10}H_{16}$	Monoterpenes (e.g., limonene*, α-Pinene*)	156±105	60206, 17107	5.1E-01±9.0E-01 (0.79)	4.3E-01±6.9E-01 (0.87)	1.3E-01±2.3E-01 (0.85)	1.4E+01±2.2E+01 (0.94)
C_4H_8O	MEK, THF, Cyclopropyl carbinol*	126±82	41369, 293752	4.3E-01±7.3E-01 (0.79)	3.7E-01±5.6E-01 (0.84)	1.1E-01±1.8E-01 (0.93)	1.2E+01±1.8E+01 (0.85)
$C_5H_{10}O_2$	Isopropyl acetate*, n-propyl acetate*	114±106	2845, 5831	4.4E-01±8.3E-01 (0.61)	3.7E-01±6.5E-01 (0.69)	1.1E-01±2.1E-01 (0.69)	1.2E+01±2.1E+01 (0.58)
$C_5H_8O_2$	Methyl methacrylate*	108±121	1102, -	4.1E-01±8.8E-01 (0.45)	3.5E-01±7.0E-01 (0.37)	1.1E-01±2.2E-01 (0.5)	1.1E+01±2.2E+01 (0.41)
$C_6H_{12}O_2$	Butyl acetate*	103±138	74432, 62692	4.9E-01±1.0E+00 (0.76)	4.1E-01±8.1E-01 (0.77)	1.3E-01±2.6E-01 (0.87)	1.3E+01±2.6E+01 (0.83)
$C_8H_8O_2$	Methyl benzoate*	92±15		1.1E-01±1.6E-01 (0.72)	9.1E-02±1.2E-01 (0.75)	2.8E-02±4.1E-02 (0.78)	3.0E+00±3.8E+00 (0.79)
$C_8H_{16}O_2$	Caprylic acid* (i.e., Octanoic acid)	87±47	5281, -	2.5E-01±4.2E-01 (0.81)	2.1E-01±3.2E-01 (0.92)	6.5E-02±1.1E-01 (0.92)	6.9E+00±1.0E+01 (0.95)
$C_3H_8O_2$	2-Methoxy ethanol, propylene glycol*	82±51	240692, -	2.9E-01±4.7E-01 (0.71)	2.4E-01±3.6E-01 (0.71)	7.5E-02±1.2E-01 (0.85)	7.9E+00±1.1E+01 (0.77)
$C_9H_{18}O_2$	Methyl octanoate, Nonanoic acid*	77±24		1.4E-01±2.3E-01 (0.79)	1.2E-01±1.7E-01 (0.9)	3.7E-02±5.7E-02 (0.9)	3.9E+00±5.4E+00 (0.94)
C_7H_6O	Benzaldehyde*	76±37	142, 2	2.1E-01±3.4E-01 (0.83)	1.8E-01±2.6E-01 (0.88)	5.4E-02±8.6E-02 (0.88)	5.7E+00±8.2E+00 (0.93)
$C_{15}H_{24}$	Sesquiterpenes (e.g., β-Caryophyllene)	70±11		7.3E-02±1.2E-01 (0.73)	6.2E-02±8.6E-02 (0.83)	1.9E-02±2.9E-02 (0.78)	2.0E+00±2.7E+00 (0.9)
$C_6H_{12}O$	2-Hexanone*, 4-Methyl-2-pentanone	59±42	6162, 16527	2.0E-01±3.6E-01 (0.83)	1.7E-01±2.8E-01 (0.84)	5.3E-02±9.0E-02 (0.92)	5.6E+00±8.8E+00 (0.91)
$C_7H_6O_2$	Benzoic acid*	59±9		5.8E-02±9.0E-02 (0.48)	4.9E-02±6.7E-02 (0.39)	1.5E-02±2.2E-02 (0.4)	1.6E+00±2.1E+00 (0.45)
C_4H_6O	MVK, MACR	58±39		1.9E-01±3.3E-01 (0.83)	1.6E-01±2.5E-01 (0.87)	4.9E-02±8.3E-02 (0.94)	5.1E+00±8.0E+00 (0.94)
$C_8H_{14}O_2$	Cyclohexyl acetate	43±20		1.2E-01±2.0E-01 (0.81)	1.0E-01±1.5E-01 (0.89)	3.2E-02±4.9E-02 (0.95)	3.4E+00±4.7E+00 (0.95)
$C_9H_{10}O_2$	Benzyl acetate	39±19	7, -	1.0E-01±1.7E-01 (0.82)	8.8E-02±1.3E-01 (0.89)	2.7E-02±4.4E-02 (0.87)	2.9E+00±4.2E+00 (0.95)
$C_6H_{14}O_3$	Dipropylene glycol	36±28	41085, 116574	1.4E-01±2.4E-01 (0.65)	1.2E-01±1.9E-01 (0.71)	3.6E-02±6.1E-02 (0.7)	3.8E+00±5.9E+00 (0.8)
$C_4H_{10}O_3$	Diethylene glycol	32±17	7026, 122315	8.9E-02±1.5E-01 (0.84)	7.5E-02±1.2E-01 (0.87)	2.3E-02±3.8E-02 (0.91)	2.4E+00±3.7E+00 (0.92)
$C_{10}H_{20}O$	Menthol, Decanal*	31±18	971, 0.06	9.4E-02±1.6E-01 (0.77)	7.9E-02±1.2E-01 (0.89)	2.4E-02±4.0E-02 (0.9)	2.6E+00±3.8E+00 (0.96)
C_5H_8O	Cyclopentanone	30±16		8.4E-02±1.4E-01 (0.84)	7.1E-02±1.1E-01 (0.9)	2.2E-02±3.5E-02 (0.95)	2.3E+00±3.4E+00 (0.95)
$C_6H_{14}O_2$	2-Butoxyethanol*, 1-propoxy-2-propanol*	23±19	107758, 79520	8.9E-02±1.6E-01 (0.8)	7.5E-02±1.2E-01 (0.87)	2.3E-02±3.9E-02 (0.91)	2.4E+00±3.8E+00 (0.9)
$C_8H_{24}O_4Si_4$	D4 siloxane*	23±3	12872, 102213	2.3E-02±3.6E-02 (0.38)	2.0E-02±2.7E-02 (0.48)	6.0E-03±8.9E-03 (0.48)	6.4E-01±8.5E-01 (0.59)
$C_{16}H_{30}O_4$	TXIB*	18±4	- , 2496	2.6E-02±4.2E-02 (0.73)	2.2E-02±3.2E-02 (0.83)	6.8E-03±1.1E-02 (0.75)	7.2E-01±1.0E+00 (0.86)

$C_{10}H_{12}O_2$	Eugenol	16±5	45, -	3.1E-02±4.9E-02 (0.82)	2.6E-02±3.7E-02 (0.85)	7.9E-03±1.2E-02 (0.91)	8.4E-01±1.2E+00 (0.92)
$C_9H_{20}O_3$	Dipropylene glycol propyl ether	16±4	4150, 6578	2.3E-02±3.8E-02 (0.65)	2.0E-02±2.9E-02 (0.71)	6.1E-03±9.5E-03 (0.62)	6.4E-01±9.1E-01 (0.73)
$C_{12}H_{16}O_3$	2-Phenoxyethyl isobutyrate	16±2		1.6E-02±2.4E-02 (0.73)	1.3E-02±1.8E-02 (0.76)	4.1E-03±5.9E-03 (0.79)	4.4E-01±5.6E-01 (0.83)
$C_{10}H_{30}O_5Si_5$	D5 siloxane*	16±15	272778, 357202	6.7E-02±1.2E-01 (0.7)	5.7E-02±9.6E-02 (0.82)	1.7E-02±3.1E-02 (0.82)	1.8E+00±3.0E+00 (0.9)
$C_{12}H_{14}O_4$	Diethyl phthalate	15±3	22898, 22923	2.3E-02±3.4E-02 (0.64)	1.9E-02±2.5E-02 (0.7)	5.9E-03±8.4E-03 (0.65)	6.2E-01±7.8E-01 (0.71)
C_7H_8O	Benzyl alcohol	14±6	17138, -	3.6E-02±5.9E-02 (0.85)	3.1E-02±4.5E-02 (0.92)	9.5E-03±1.5E-02 (0.92)	--
$C_8H_{14}O$	6-Methyl 5-hepten-2-one	14±7		4.1E-02±6.6E-02 (0.81)	3.4E-02±5.0E-02 (0.89)	1.1E-02±1.6E-02 (0.96)	1.1E+00±1.6E+00 (0.96)
$C_8H_8O_3$	Methyl paraben	14±4		2.4E-02±3.9E-02 (0.83)	2.1E-02±2.9E-02 (0.86)	6.3E-03±9.7E-03 (0.83)	6.7E-01±9.2E-01 (0.87)
$C_4H_{10}O_2$	1-Methoxy-2-propanol	13±8	3405, 2405	4.1E-02±7.1E-02 (0.78)	3.5E-02±5.4E-02 (0.85)	1.1E-02±1.8E-02 (0.89)	1.1E+00±1.7E+00 (0.89)
$C_5H_4O_2$	Furfural*	13±6	- , 0.01	3.4E-02±5.7E-02 (0.71)	2.9E-02±4.3E-02 (0.62)	8.8E-03±1.4E-02 (0.56)	9.3E-01±1.4E+00 (0.66)
$C_6H_{10}O$	Cyclohexanone	12±6	10017, 8214	3.6E-02±5.9E-02 (0.84)	3.0E-02±4.5E-02 (0.91)	9.4E-03±1.5E-02 (0.96)	9.9E-01±1.4E+00 (0.92)
$C_6H_{12}O_3$	PGMEA, 2-Ethoxyethyl acetate	12±11	384, 106653	4.7E-02±8.8E-02 (0.78)	4.0E-02±6.8E-02 (0.76)	1.2E-02±2.2E-02 (0.9)	1.3E+00±2.2E+00 (0.86)
$C_6H_6O_3$	Maltol	11±3		1.3E-02±2.3E-02 (0.59)	1.1E-02±1.7E-02 (0.44)	3.4E-03±5.6E-03 (0.42)	3.6E-01±5.4E-01 (0.49)
C_8H_8O	Acetophenone*	10±6	4, -	3.2E-02±5.5E-02 (0.81)	2.7E-02±4.2E-02 (0.85)	8.4E-03±1.4E-02 (0.89)	8.8E-01±1.3E+00 (0.9)
C_5H_9NO	Methyl pyrrolidone	9±3	12749, 15452	1.9E-02±3.1E-02 (0.72)	1.6E-02±2.3E-02 (0.78)	5.0E-03±7.7E-03 (0.77)	5.3E-01±7.4E-01 (0.78)
$C_8H_{10}O_2$	Phenoxyethanol*	9±3	9851, 0.25	1.7E-02±2.9E-02 (0.78)	1.5E-02±2.2E-02 (0.84)	4.5E-03±7.2E-03 (0.86)	4.8E-01±6.9E-01 (0.91)
$C_8H_{18}O_3$	2-(2-Butoxyethoxy)ethanol, DGBE	8±4	48389, 68370	2.1E-02±3.5E-02 (0.85)	1.8E-02±2.7E-02 (0.91)	5.4E-03±8.7E-03 (0.89)	5.7E-01±8.4E-01 (0.94)
$C_{10}H_{10}O_4$	Dimethyl phthalate	7±1	70, -	9.1E-03±1.5E-02 (0.62)	7.7E-03±1.1E-02 (0.62)	2.4E-03±3.6E-03 (0.55)	2.5E-01±3.4E-01 (0.65)
$C_{12}H_{24}O_3$	Texanol*	7±4	267615, 197658	2.0E-02±3.5E-02 (0.57)	1.7E-02±2.7E-02 (0.74)	5.3E-03±8.7E-03 (0.67)	5.6E-01±8.4E-01 (0.74)
$C_9H_{10}O_3$	Ethyl paraben	6±1		7.0E-03±1.1E-02 (0.84)	5.9E-03±8.2E-03 (0.84)	1.8E-03±2.7E-03 (0.85)	1.9E-01±2.6E-01 (0.9)
$C_{11}H_{14}O_3$	Butyl paraben	6±1		8.5E-03±1.3E-02 (0.71)	7.2E-03±9.4E-03 (0.74)	2.2E-03±3.1E-03 (0.8)	2.3E-01±2.9E-01 (0.76)
$C_6H_{10}O_3$	Ethyl acetoacetate	4±2		1.3E-02±2.2E-02 (0.85)	1.1E-02±1.6E-02 (0.87)	3.4E-03±5.4E-03 (0.93)	3.6E-01±5.2E-01 (0.91)
$C_{10}H_{12}O$	Benzyl acetone	4±2		1.0E-02±1.7E-02 (0.85)	8.5E-03±1.3E-02 (0.91)	2.6E-03±4.2E-03 (0.94)	2.8E-01±4.1E-01 (0.97)
$C_7H_{12}O_4$	Pentadioic acid, dimethyl ester	4±1	4942, 28232	7.2E-03±1.1E-02 (0.8)	6.1E-03±8.5E-03 (0.84)	1.9E-03±2.8E-03 (0.87)	2.0E-01±2.7E-01 (0.89)
$C_{10}H_{12}O_3$	Propyl paraben	4±1		6.3E-03±1.0E-02 (0.54)	5.3E-03±7.7E-03 (0.46)	1.6E-03±2.5E-03 (0.42)	1.7E-01±2.4E-01 (0.51)
$C_{10}H_{20}O_2$	Hydroxycitronellal	3±1		5.3E-03±8.4E-03 (0.78)	4.5E-03±6.3E-03 (0.88)	1.4E-03±2.1E-03 (0.92)	1.5E-01±2.0E-01 (0.95)
$C_8H_{18}O_2$	Ethylene glycol hexyl ether*, 1,2-Octanediol	2±1	15836, 8544	5.8E-03±9.6E-03 (0.8)	4.9E-03±7.3E-03 (0.88)	1.5E-03±2.4E-03 (0.87)	1.6E-01±2.3E-01 (0.94)
$C_3H_8O_3$	Glycerol	1±0.5	148441, 1046753	3.0E-03±4.9E-03 (0.66)	2.6E-03±3.7E-03 (0.69)	7.9E-04±1.2E-03 (0.75)	8.3E-02±1.2E-01 (0.74)
$C_6H_{14}O_4$	Triethylene glycol	1±0.3	1718, 1053	2.1E-03±3.4E-03 (0.47)	1.8E-03±2.6E-03 (0.45)	5.5E-04±8.4E-04 (0.4)	5.8E-02±8.0E-02 (0.51)