Supplement of Atmos. Chem. Phys., 20, 9753–9770, 2020
https://doi.org/10.5194/acp-20-9753-2020-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Source characterization of volatile organic compounds measured by proton-transfer-reaction time-of-flight mass spectrometers in Delhi, India

Liwei Wang et al.

Correspondence to: Sachchida N. Tripathi (snt@iitk.ac.in) and André S. H. Prévôt (andre.prevot@psi.ch)

Concentration weighted trajectory (CWT) analysis

Backward-trajectory analysis was performed using Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model. The meteorological fields were obtained from the National Centers for Environmental Prediction (NCEP) Global Data Assimilation System (GDAS). (Stein et al., 2015) We performed hourly resolution back-trajectories for 6 hours, 12 hours, 24 hours and 48 hours. Owing to the short distance between the two sites (20 km) and short lifetime of VOCs, the 6-hour and 12-hour back-trajectories were found to be a good representation of the air mass transport between the two sites. The concentration weighted trajectory (CWT) analysis is widely used to reveal the potential source regions and spatial distribution of pollutants (Zheng et al., 2019). In this paper, the CWT analysis is based on the back-trajectories with an arriving height at 100 m above sea level for 6 hrs. Here, we utilized an Igor based tool, Zefir (Petit et al., 2017), to explore the CWT plots with a cell resolution of $0.2^{\circ} \times 0.2^{\circ}$.

Reference

Petit, J. E., Favez, O., Albinet, A., and Canonaco, F.: A user-friendly tool for comprehensive evaluation of the geographical origins of atmospheric pollution: Wind and trajectory analyses, Environmental Modelling & Software, 88, 183-187, https://doi.org/10.1016/j.envsoft.2016.11.022, 2017.

Stein, A. F., Draxler, R. R., Rolph, G. D., Stunder, B. J. B., Cohen, M. D., and Ngan, F.: NOAA's HYSPLIT Atmospheric Transport and Dispersion Modeling System, Bulletin of the American Meteorological Society, 96, 2059-2077, 10.1175/bams-d-14-00110.1, 2015.

Zheng, H., Kong, S., Wu, F., Cheng, Y., Niu, Z., Zheng, S., Yang, G., Yao, L., Yan, Q., Wu, J., Zheng, M., Chen, N., Xu, K., Yan, Y., Liu, D., Zhao, D., Zhao, T., Bai, Y., Li, S., and Qi, S.: Intra-regional transport of black carbon between the south edge of the North China Plain and central China during winter haze episodes, Atmos. Chem. Phys., 19, 4499-4516, 10.5194/acp-19-4499-2019, 2019.

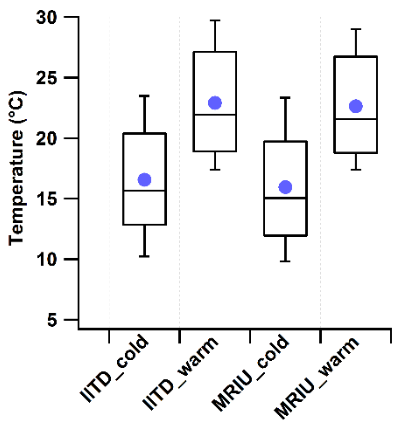

Fig. S1 Box-whisker plots of temperature during the cold and warm periods at the two sites. The comparisons of temperature change during different periods, and at each site are based on the periods when VOC measurements exist.

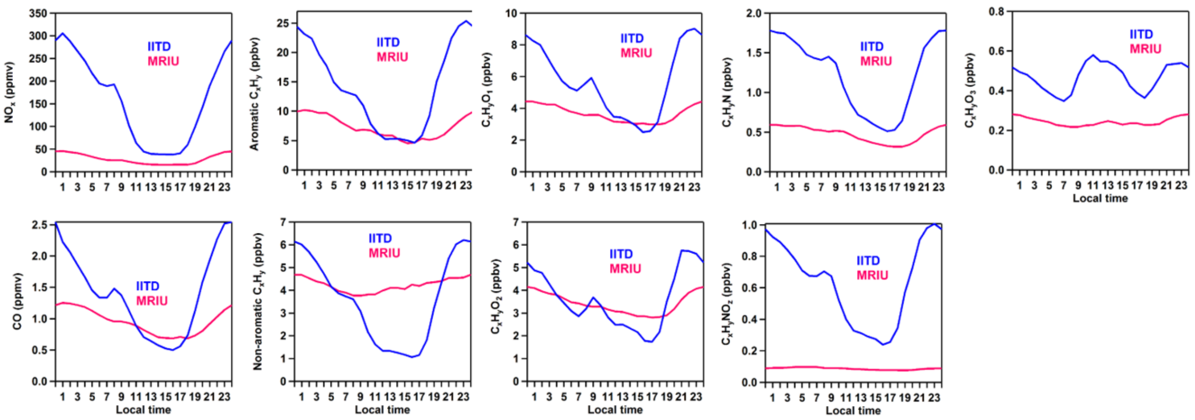

Fig. S2 Diurnal plots of averaged mixing ratio of NO_x, CO and each VOC family at each site.

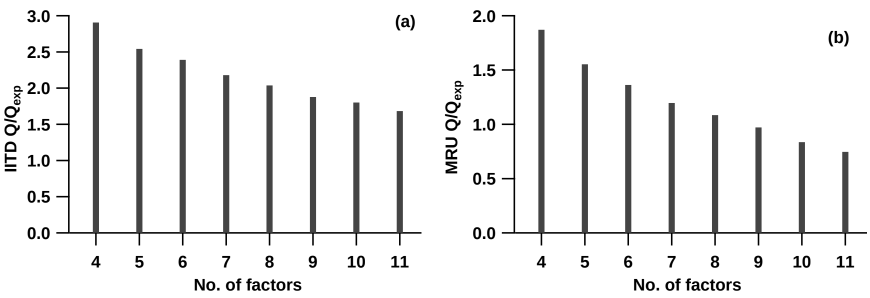

Fig. S3 Q/Q_{exp} plots vs number of factors of (a) IITD and (b) MRIU.

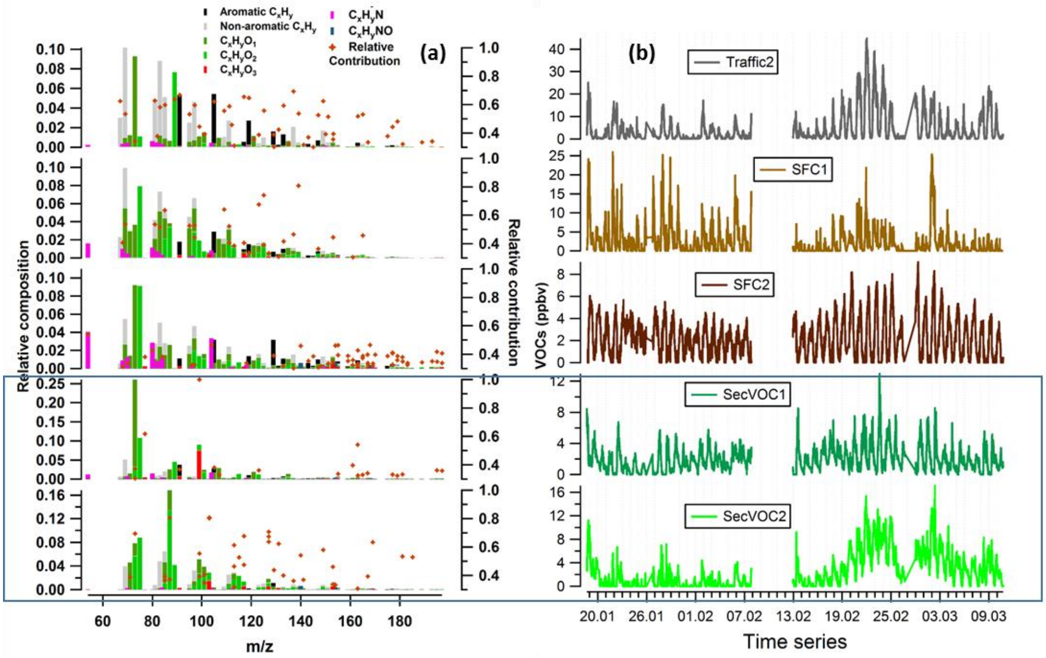

Fig. S4 PMF results at IITD with the input of 154 ions (excluding $C_6H_6H^+$, $C_7H_8H^+$, $C_8H_{10}H^+$, and $C_9H_{12}H^+$), showing (a) factor profiles (b) factor time series. The selected secondary factors are labeled in the blue box.

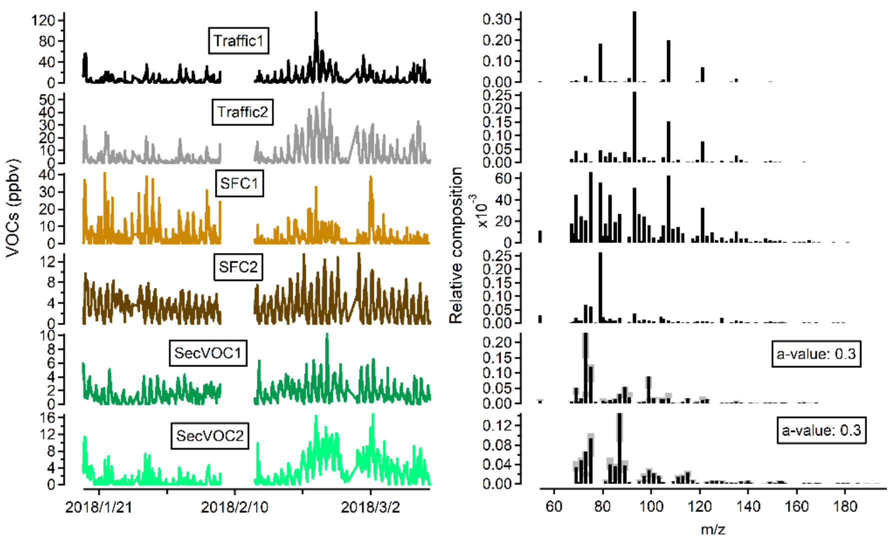

Fig. S5 PMF results at IITD with the a-value=0.3, showing on the left the factor time series, and on the right the factor profiles. The shaded area spans the lower and higher constraints and the comparison between the gray area and the factor profile indicates in which direction the solution was pulled during the ME-2 run.

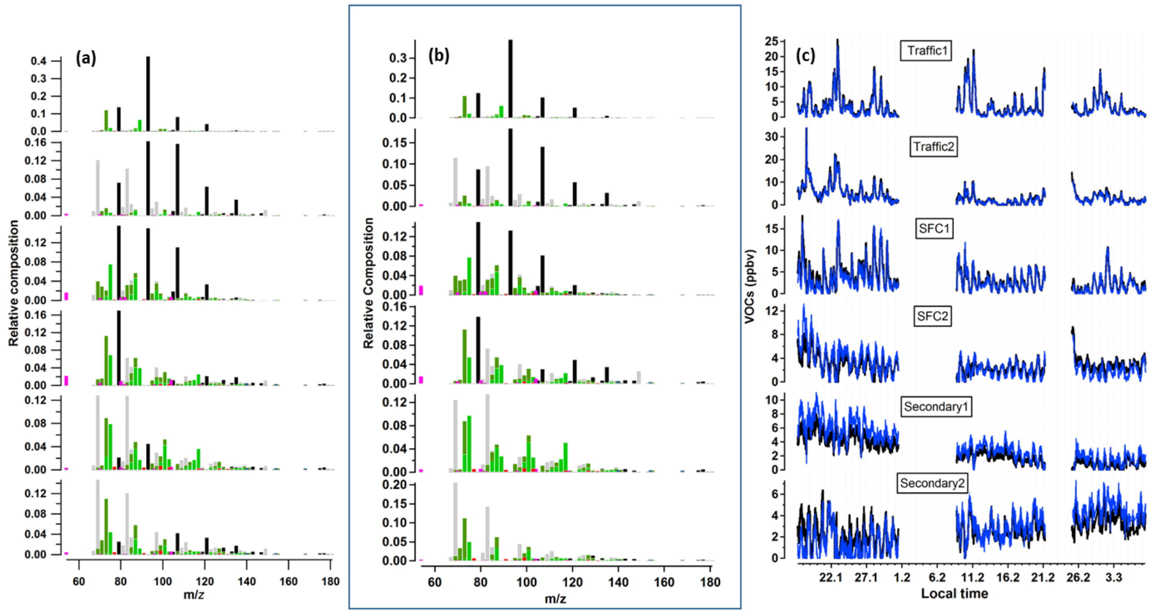

Fig. S6 (a) Factor profiles of raw PMF result at MRIU. (b) Factor profiles of PMF result at MRIU by constraining the two secondary factors as applied at IITD. (c) Factor time series of the two PMF results at MRIU, with the blue lines showing the unconstrained PMF results (corresponds to a), and the black lines showing the constrained results (b).

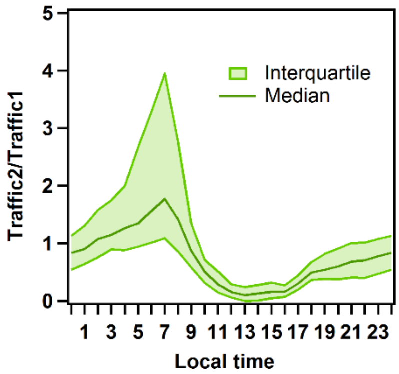

Fig.S7 Diurnal plot of the ratio of Traffic2 to Traffic1 at IITD. The shaded area represents the interquartile range.

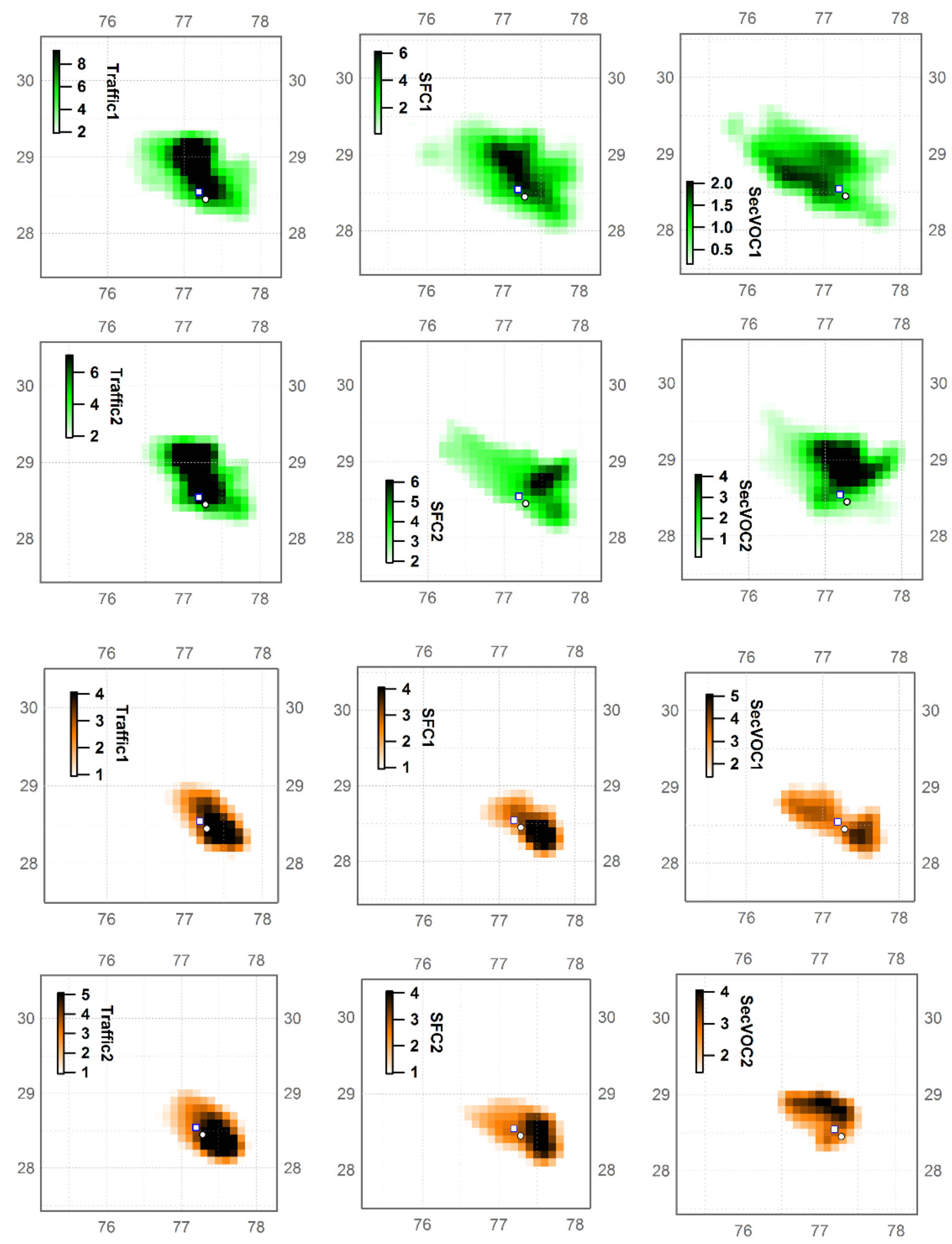

Fig. S8 Concentration weighted trajectory (CWT) plots of PMF factors with the back-trajectory calculated for 6 hours at both sites. The green plots represent the IITD factors and the gold plots are the MRIU factors. In each plot, the white square represents the IITD site and the white circle represents the MRIU site.

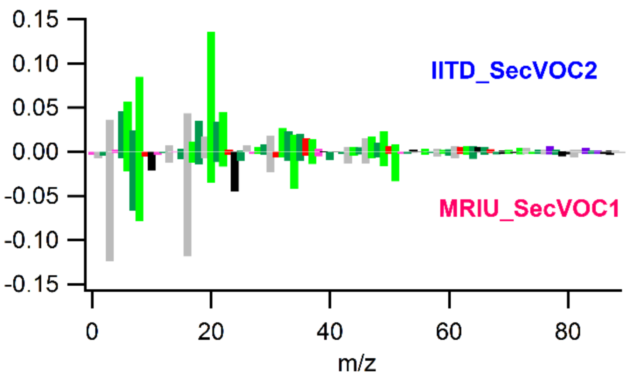

Fig. S9 Comparison of the factor spectra of IITD SecVOC2 and MRIU SecVOC1.

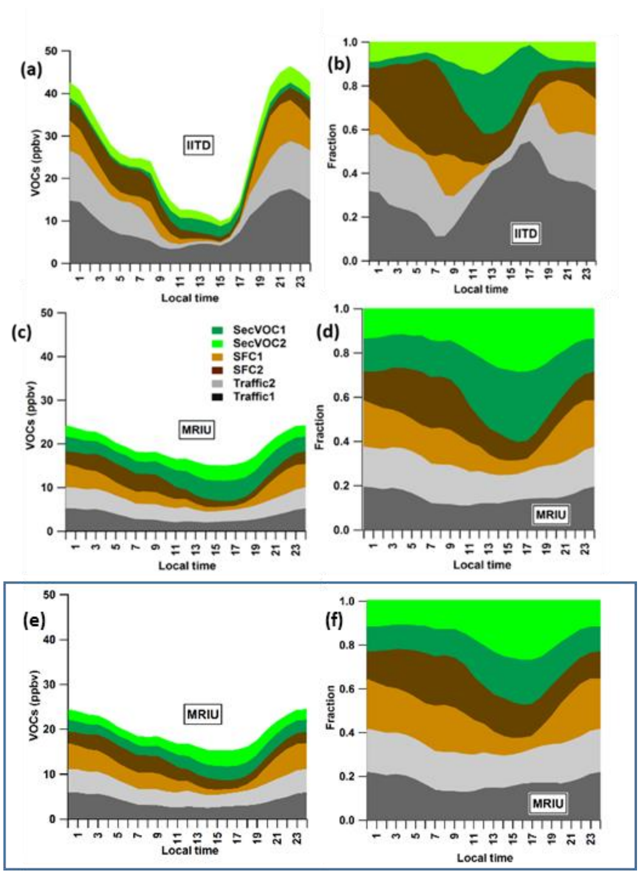

Fig. S10 Diurnal patterns of factor concentrations and contributions (a) at IITD, (b) raw result at MRIU, and (c) constrained result at MRIU.

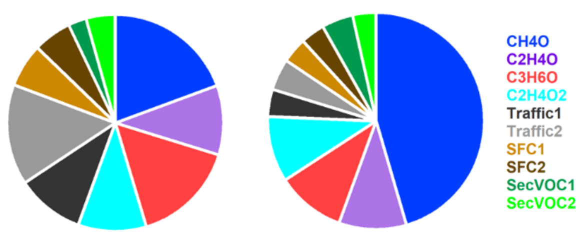

Fig. S11. Volume contributions of CH3OH, C2H4O, C3H6O, C2H4O2 and the six PMF factors at the two sites. The left pie represents the IITD site and the right pie the MRIU site.

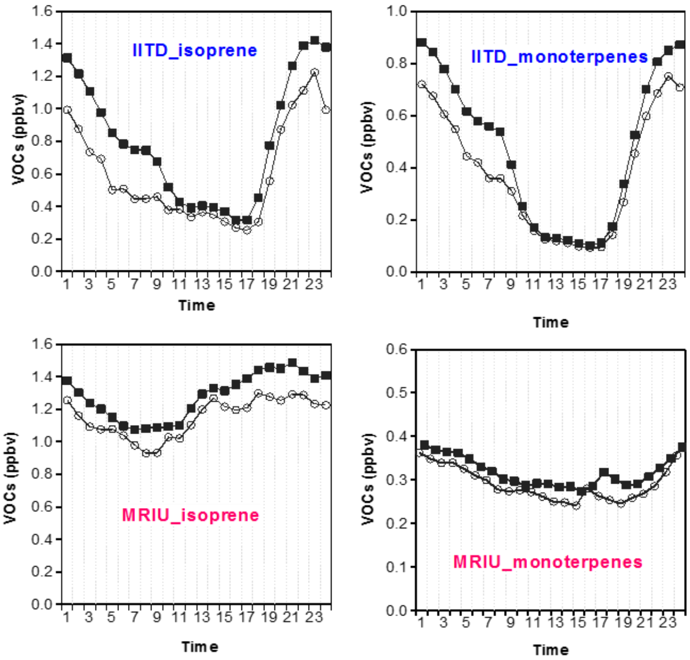

Fig. S12 Diurnal patterns of isoprene and monoterpenes at the two sites. The squares represent the mean values and the circles the median values.

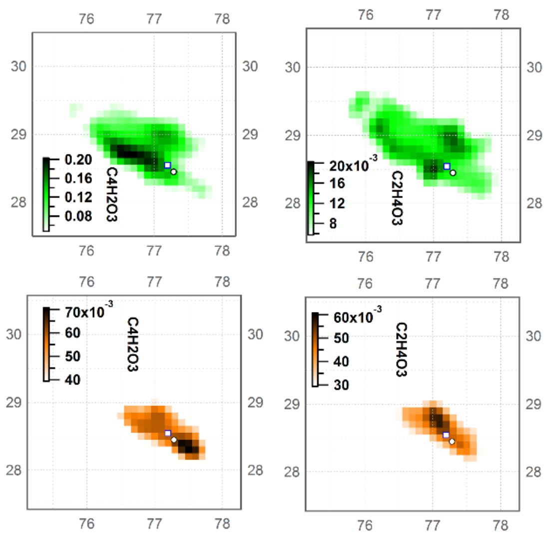

Fig. S13 CWT plots of maleic anhydride and PAN with the 6-hour back-trajectories at both sites. The green plots represent the IITD factors and the gold plots the MRIU factors. In each plot, the white square represents the IITD site and the white circle represents the MRIU site.

Table S1 List of ions and averaged mixing ratios included in the PMF analysis at IITD.

Ion exact m/z (Th)	Ion formula	Averaged mixing ratio (ppbv)
54.034	C3H3NH$^+$	0.17
67.054	C5H6H$^+$	0.23
68.049	C4H5NH$^+$	0.065
69.033	C4H4OH$^+$	0.26
69.070	C5H8H$^+$	0.80
70.065	C4H7NH$^+$	0.087
71.049	C4H6OH$^+$	0.32
73.028	C3H4O2H$^+$	0.25
73.065	C4H8OH$^+$	1.3
75.044	C3H6O2H$^+$	0.92
77.023	C2H4O3H$^+$	0.017
79.054	C6H6H$^+$	2.8
80.049	C5H5NH$^+$	0.15
81.033	C5H4OH$^+$	0.10
81.070	C6H8H$^+$	0.33
82.065	C5H7NH$^+$	0.064
83.049	C5H6OH$^+$	0.26
83.086	C6H10H$^+$	0.60
84.081	C5H9NH$^+$	0.068
85.028	C4H4O2H$^+$	0.094
85.065	C5H8OH$^+$	0.24
85.101	C6H12H$^+$	0.34
87.044	C4H6O2H$^+$	0.46
87.080	C5H10OH$^+$	0.24
89.060	C4H8O2H$^+$	0.70
91.039	C3H6O3H$^+$	0.064
91.054	C7H6H$^+$	0.38
93.070	C7H8H$^+$	5.2
95.049	C6H6OH$^+$	0.17
95.086	C7H10H$^+$	0.17
96.081	C6H9NH$^+$	0.021
97.028	C5H4O2H$^+$	0.14
97.065	C6H8OH$^+$	0.15
97.101	C7H12H$^+$	0.30
99.008	C4H2O3H$^+$	0.16
99.044	C5H6O2H$^+$	0.18
99.080	C6H10OH$^+$	0.15
101.060	C5H8O2H$^+$	0.15
101.096	C6H12OH$^+$	0.16
103.039	C4H6O3H$^+$	0.055
103.075	C5H10O2H$^+$	0.049
104.049	C7H5NH$^+$	0.16
105.033	C7H4OH$^+$	0.091
105.070	C8H8H$^+$	0.38
107.049	C7H6OH$^+$	0.22
107.086	C8H10H$^+$	3.1
109.065	C7H8OH$^+$	0.065
109.101	C8H12H$^+$	0.078
. 111.044	C6H6O2H$^+$	0.086
111.080	C7H10OH$^+$	0.081
111.117	C8H14H$^+$	0.17
112.112	C7H13NH$^+$	0.022
113.060	C6H8O2H$^+$	0.077
113.096	C7H12OH$^+$	0.061
113.132	C8H16H$^+$	0.019
115.075	C6H10O2H$^+$	0.12
117.055	C5H8O3H$^+$	0.038
117.070	C9H8H$^+$	0.028
117.091	C6H12O2H$^+$	0.035
118.065	C8H7NH$^+$	0.028
119.049	C8H6OH$^+$	0.043
119.086	C9H10H$^+$	0.18
121.065	C8H8OH$^+$	0.16
121.101	C9H12H$^+$	1.3
123.044	C7H6O2H$^+$	0.073
123.080	C8H10OH$^+$	0.031
123.117	C9H14H$^+$	0.048
125.060	C7H8O2H$^+$	0.042
125.096	C8H12OH$^+$	0.029
125.132	C9H16H$^+$	0.064
127.039	C6H6O3H$^+$	0.022
127.075	C7H10O2H$^+$	0.027
127.112	C8H14OH$^+$	0.027
127.148	C9H18H$^+$	0.015
129.070	C10H8H$^+$	0.17
129.127	C8H16OH$^+$	0.033
131.070	C6H10O3H$^+$	0.012
131.086	C10H10H$^+$	0.021
131.143	C8H18OH$^+$	0.009
133.028	C8H4O2H$^+$	0.016
133.065	C9H8OH$^+$	0.030
133.101	C10H12H$^+$	0.088
135.044	C8H6O2H$^+$	0.036
135.080	C9H10OH$^+$	0.084
135.117	C10H14H$^+$	0.44
137.060	C8H8O2H$^+$	0.035
137.096	C9H12OH$^+$	0.022
137.132	C10H16H$^+$	0.14
139.075	C8H10O2H$^+$	0.016
139.112	C9H14OH$^+$	0.026
139.148	C10H18H$^+$	0.025
140.034	C6H5NO3H$^+$	0.037
141.127	C9H16OH$^+$	0.017
141.164	C10H20H$^+$	0.012
143.086	C11H10H$^+$	0.040
145.065	C10H8OH$^+$	0.008
145.101	C11H12H$^+$	0.012

147.080	$C10H10OH^+$	0.034
147.117	$C11H14H^+$	0.049
148.112	$C10H13NH^+$	0.015
149.060	$C9H8O2H^+$	0.020
149.096	$C10H12OH^+$	0.038
149.132	$C11H16H^+$	0.11
150.128	$C10H15NH^+$	0.019
151.039	$C8H6O3H^+$	0.012
151.075	$C9H10O2H^+$	0.017
151.112	$C10H14OH^+$	0.014
151.148	$C11H18H^+$	0.031
153.055	$C8H8O3H^+$	0.035
153.091	$C9H12O2H^+$	0.014
153.127	$C10H16OH^+$	0.046
153.164	$C11H20H^+$	0.017
154.050	$C7H7NO3H^+$	0.034
155.070	$C8H10O3H^+$	0.011
155.086	$C12H10H^+$	0.013
155.143	$C10H18OH^+$	0.016
155.179	$C11H22H^+$	0.012
159.080	$C11H10OH^+$	0.006
159.117	$C12H14H^+$	0.008
161.060	$C10H8O2H^+$	0.012
161.096	$C11H12OH^+$	0.010
163.039	$C9H6O3H^+$	0.013
163.075	$C10H10O2H^+$	0.010
163.112	$C11H14OH^+$	0.010
163.133	$C8H18O3H^+$	0.011
163.148	$C12H18H^+$	0.035
165.055	$C9H8O3H^+$	0.005
165.091	$C10H12O2H^+$	0.014
165.127	$C11H16OH^+$	0.008
165.164	$C12H20H^+$	0.024
167.070	$C9H10O3H^+$	0.006
167.107	$C10H14O2H^+$	0.005
167.143	$C11H18OH^+$	0.008
167.179	$C12H22H^+$	0.011
168.066	$C8H9NO3H^+$	0.018
169.086	$C9H12O3H^+$	0.005
169.122	$C10H16O2H^+$	0.009
169.159	$C11H20OH^+$	0.008
169.195	$C12H24H^+$	0.010
170.096	$C12H11NH^+$	0.006
175.148	$C13H18H^+$	0.016
177.091	$C11H12O2H^+$	0.005
177.127	$C12H16OH^+$	0.008
177.164	$C13H20H^+$	0.020
179.086	$C14H10H^+$	0.006
179.143	$C12H18OH^+$	0.006
179.179	$C13H22H^+$	0.017
181.159	$C12H20OH^+$	0.006

181.195	$C13H24H^+$	0.008
183.138	$C11H18O2H^+$	0.005
183.211	$C13H26H^+$	0.008
185.190	$C12H24OH^+$	0.005
189.091	$C12H12O2H^+$	0.008
193.159	$C13H20OH^+$	0.011
195.102	$C11H14O3H^+$	0.004
195.138	$C12H18O2H^+$	0.006
197.117	$C11H16O3H^+$	0.005
197.154	$C12H20O2H^+$	0.007

Table S2 List of ions and averaged mixing ratios included in the PMF analysis at MRIU

Ion exact m/z (Th)	Ion formula	Averaged mixing ratio (ppbv)
54.034	$C3H3NH^+$	0.15
67.054	$C5H6H^+$	0.13
69.034	$C4H4OH^+$	0.21
69.070	$C5H8H^+$	1.3
70.065	$C4H7NH^+$	0.059
71.049	$C4H6OH^+$	0.29
73.028	$C3H4O2H^+$	0.14
73.065	$C4H8OH^+$	1.3
75.044	$C3H6O2H^+$	0.90
77.023	$C2H4O3H^+$	0.050
79.054	$C6H6H^+$	1.8
80.050	$C5H5NH^+$	0.069
81.034	$C5H4OH^+$	0.043
81.070	$C6H8H^+$	0.25
82.065	$C5H7NH^+$	0.043
83.049	$C5H6OH^+$	0.16
83.086	$C6H10H^+$	1.3
85.028	$C4H4O2H^+$	0.13
85.065	$C5H8OH^+$	0.22
85.101	$C6H12H^+$	0.24
87.044	$C4H6O2H^+$	0.54
87.080	$C5H10OH^+$	0.24
89.060	$C4H8O2H^+$	0.43
91.039	$C3H6O3H^+$	0.033
93.070	$C7H8H^+$	2.6
95.049	$C6H6OH^+$	0.14
95.086	$C7H10H^+$	0.060
96.081	$C6H9NH^+$	0.026
97.028	$C5H4O2H^+$	0.12
97.065	$C6H8OH^+$	0.094
97.101	$C7H12H^+$	0.38
99.008	$C4H2O3H^+$	0.060
99.044	$C5H6O2H^+$	0.069
99.080	$C6H10OH^+$	0.16
101.060	$C5H8O2H^+$	0.25
101.096	$C6H12OH^+$	0.21
103.039	$C4H6O3H^+$	0.040
103.075	$C5H10O2H^+$	0.13
104.049	$C7H5NH^+$	0.10
105.070	$C8H8H^+$	0.17
107.049	$C7H6OH^+$	0.084
107.086	$C8H10H^+$	1.3
109.065	$C7H8OH^+$	0.033
109.101	$C8H12H^+$	0.12
111.044	$C6H6O2H^+$	0.065
111.080	$C7H10OH^+$	0.045
111.117	$C8H14H^+$	0.21
113.060	$C6H8O2H^+$	0.071
113.096	$C7H12OH^+$	0.067
115.075	$C6H10O2H^+$	0.13
117.055	$C5H8O3H^+$	0.024
117.091	$C6H12O2H^+$	0.25
118.065	$C8H7NH^+$	0.023
119.049	$C8H6OH^+$	0.023
119.086	$C9H10H^+$	0.061
121.101	$C9H12H^+$	0.61
123.044	$C7H6O2H^+$	0.039
123.080	$C8H10OH^+$	0.020
123.117	$C9H14H^+$	0.056
125.060	$C7H8O2H^+$	0.027
125.096	$C8H12OH^+$	0.038
125.132	$C9H16H^+$	0.095
127.039	$C6H6O3H^+$	0.022
127.075	$C7H10O2H^+$	0.030
127.112	$C8H14OH^+$	0.070
129.070	$C10H8H^+$	0.077
129.127	$C8H16OH^+$	0.043
131.070	$C6H10O3H^+$	0.012
133.065	$C9H8OH^+$	0.025
133.101	$C10H12H^+$	0.060
135.044	$C8H6O2H^+$	0.024
135.117	$C10H14H^+$	0.25
137.060	$C8H8O2H^+$	0.034
137.132	$C10H16H^+$	0.077
139.075	$C8H10O2H^+$	0.021
139.112	$C9H14OH^+$	0.029
139.148	$C10H18H^+$	0.038
140.034	$C6H5NO3H^+$	0.040
141.127	$C9H16OH^+$	0.028
143.086	$C11H10H^+$	0.062
147.117	$C11H14H^+$	0.056
149.132	$C11H16H^+$	0.13
153.164	$C11H20H^+$	0.023
154.050	$C7H7NO3H^+$	0.028
155.143	$C10H18OH^+$	0.018
168.066	$C8H9NO3H^+$	0.019
175.148	$C13H18H^+$	0.026
177.164	$C13H20H^+$	0.043
179.179	$C13H22H^+$	0.022
181.195	$C13H24H^+$	0.012