

Supplement of

**Source characterization of volatile organic compounds
measured by PTR-ToF-MS in Delhi, India**

Wang et al.

Correspondence to: André S. H. Prévôt and Sachchida N. Tripathi

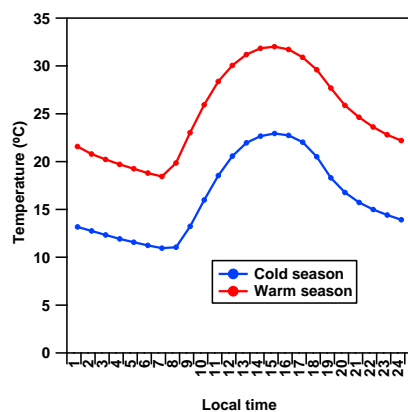


Fig. S1 Mean diurnal cycles of temperature of the cold and warm seasons

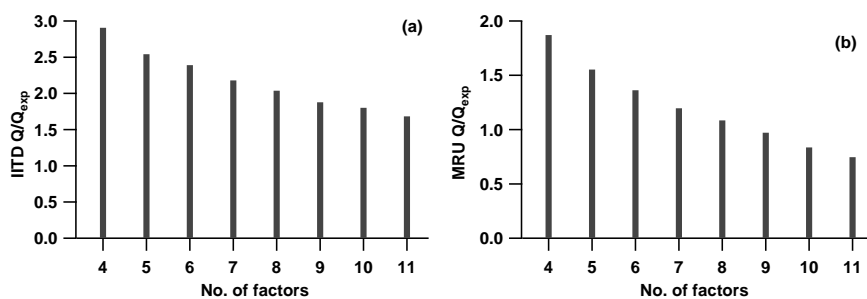


Fig. S2 Q/Q_{exp} plots vs number of factors of (a) IITD and (b) MRIU.

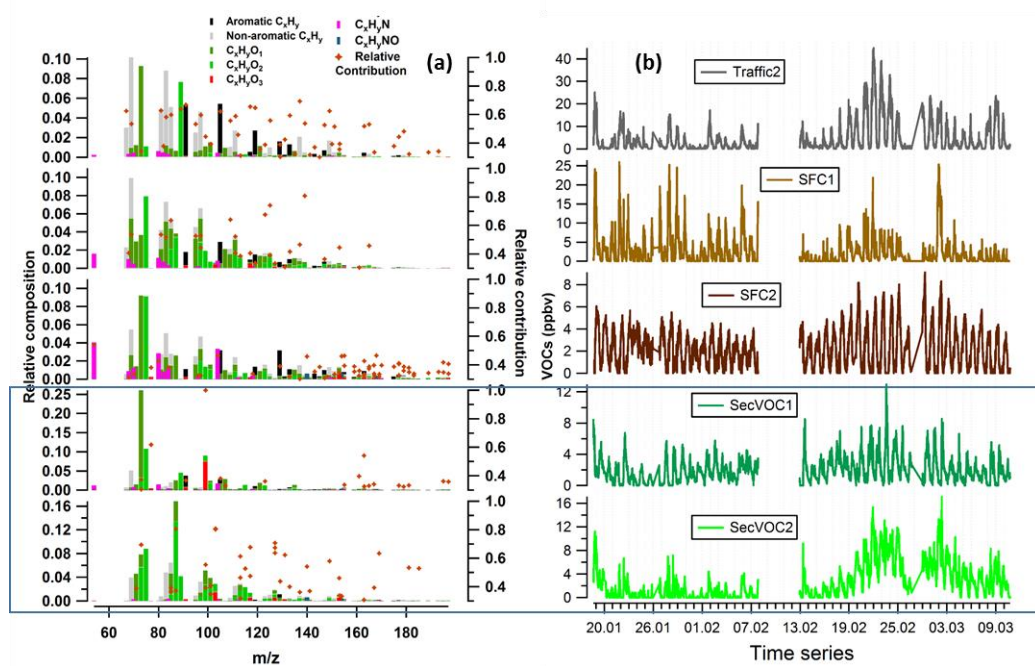


Fig. S3 PMF results at IITD with the input of 154 ions (excluding $C_6H_6H^+$, $C_7H_8H^+$, $C_8H_{10}H^+$, and $C_9H_{12}H^+$), showing (a) factor profiles (b) factor time series. The selected secondary factors are labeled in the blue box.

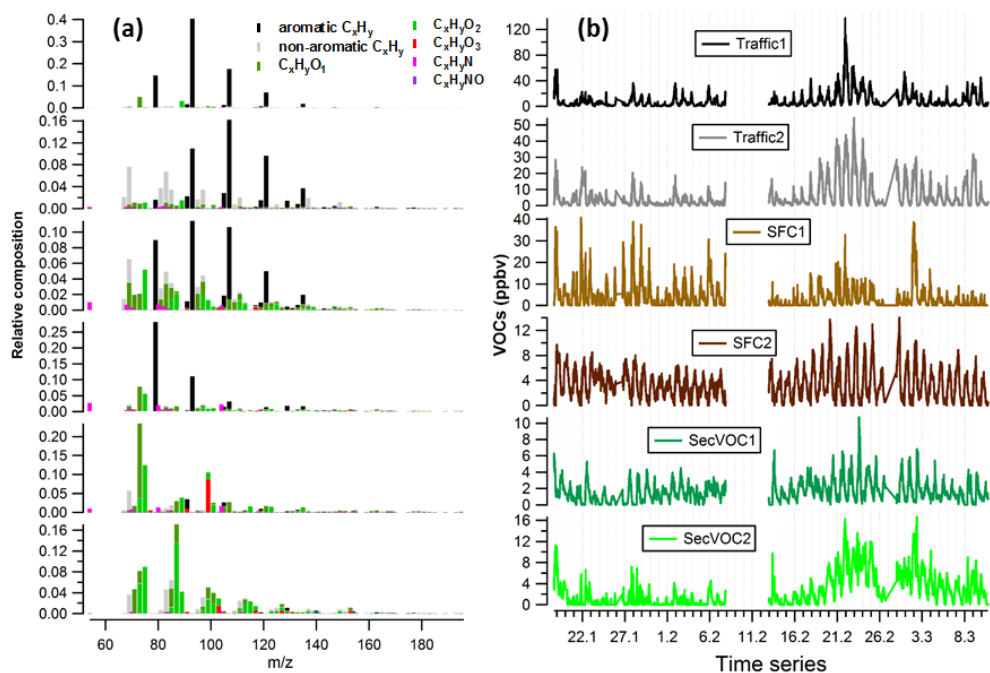


Fig. S4 Averaged PMF results at IITD with the a-value ranging from 0.1-0.3, showing (a) factor profiles (b) factor time series.

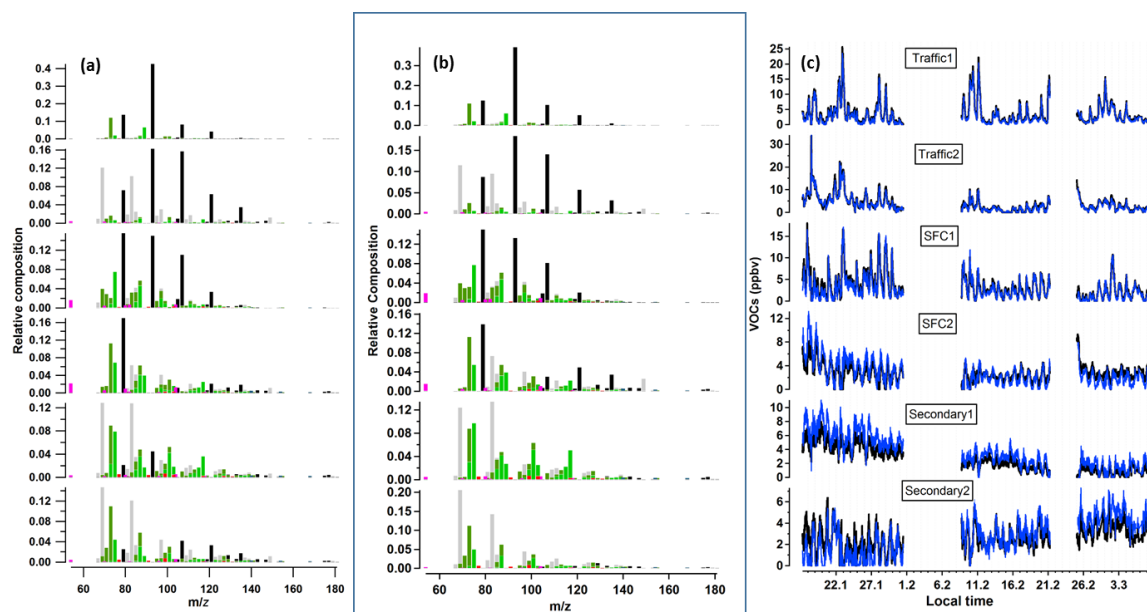


Fig. S5 (a) Factor profiles of raw PMF result at MRIU. (b) Factor profiles of PMF result at MRIU by constraining the two secondary factors as applied at IITD. (c) Factor time series of the two PMF results at MRIU, with the blue lines showing the unconstrained PMF results (corresponds to a), and the black lines showing the constrained results (b).

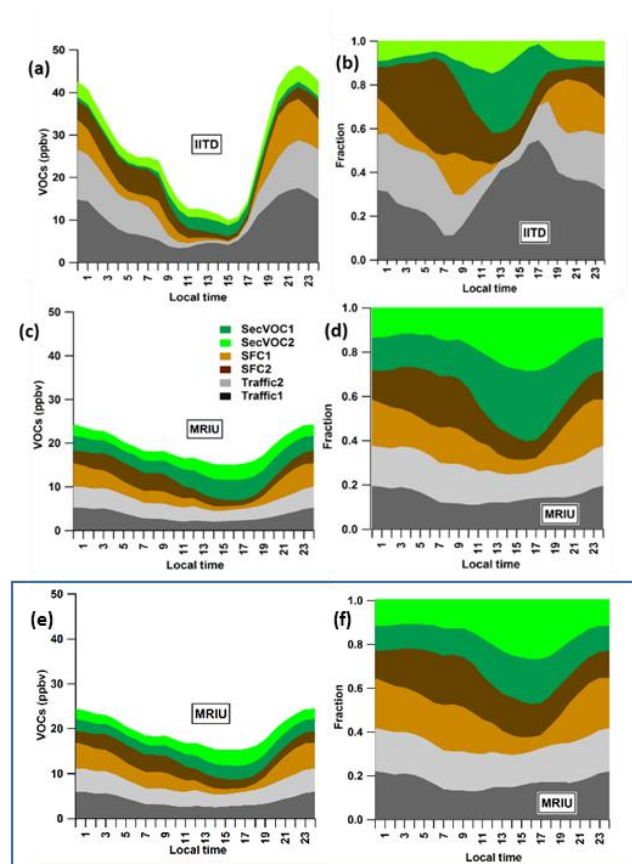


Fig. S6 Diurnal patterns of factor concentrations and contributions (a) at IITD, (b) raw result at MRIU, and (c) constrained result at MRIU.

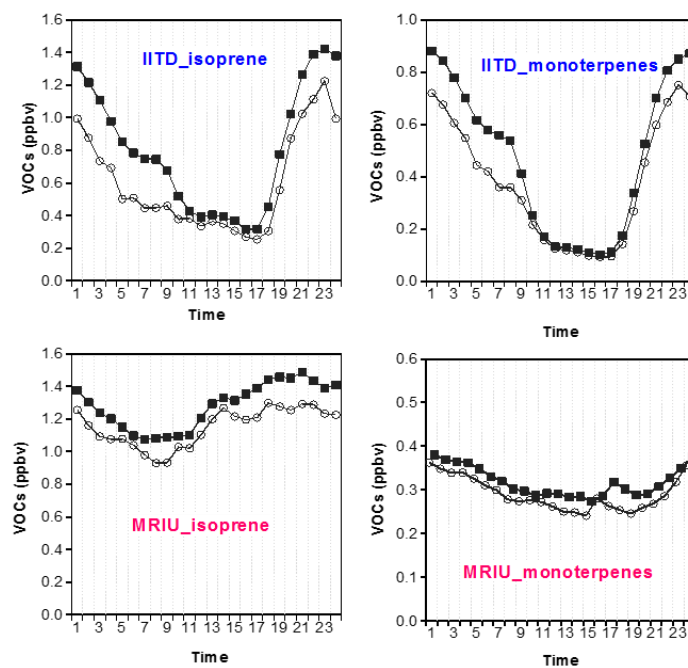


Fig. S7 Diurnal patterns of isoprene and monoterpenes at the two sites. The squares represent the mean values and the circles represent median values.

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
.	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	181.195	C13H24H ⁺	0.008
147.117	C11H14H ⁺	0.049	183.138	C11H18O2H ⁺	0.005
148.112	C10H13NH ⁺	0.015	183.211	C13H26H ⁺	0.008
149.060	C9H8O2H ⁺	0.020	185.190	C12H24OH ⁺	0.005
149.096	C10H12OH ⁺	0.038	189.091	C12H12O2H ⁺	0.008
149.132	C11H16H ⁺	0.11	193.159	C13H20OH ⁺	0.011
150.128	C10H15NH ⁺	0.019	195.102	C11H14O3H ⁺	0.004
151.039	C8H6O3H ⁺	0.012	195.138	C12H18O2H ⁺	0.006
151.075	C9H10O2H ⁺	0.017	197.117	C11H16O3H ⁺	0.005
151.112	C10H14OH ⁺	0.014	197.154	C12H20O2H ⁺	0.007
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			

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