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Reactive chlorine-, sulfur-, and nitrogen-containing volatile organic compounds impact atmospheric chemistry in the megacity of Delhi during both clean and extremely polluted seasons

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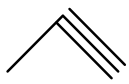
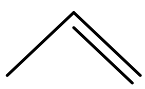
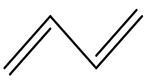
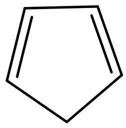
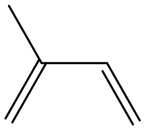
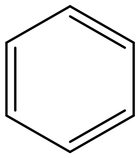
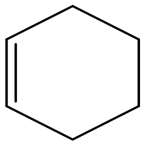
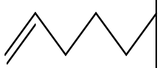
Table S1: Operational settings for PTR-TOF-MS 10 K parameters used during this deployment

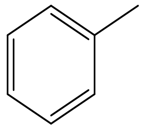
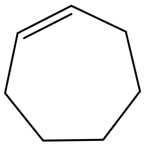
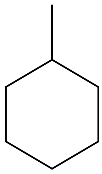
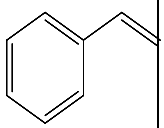
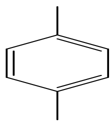
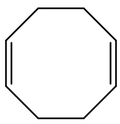
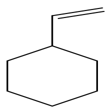
Parameters	Values
Overall drift voltage (U_{drift})	470 V
Temperature at drift tube (T_{drift})	120 ^{0}C
Pressure at drift tube (P_{drift})	3.0 mbar
Length of the drift tube (L_{drift})	9.2 cm
Extraction time (t)	26 µs
Field strength of the drift tube (E/N)	120 Td

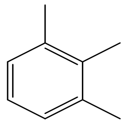
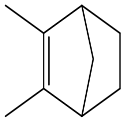
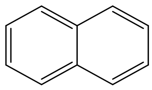
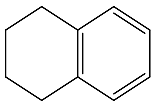
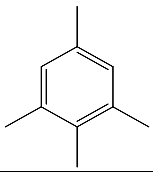
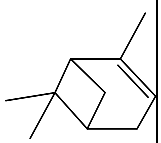
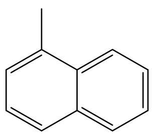
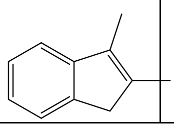
* *E* is the electric field strength (V cm^{-1}) and *N* is the gas number density (molecule cm^{-3}). 1 Td = 10^{-17} V cm^2

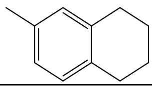
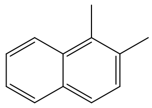
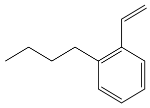
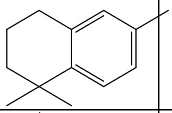
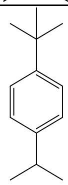
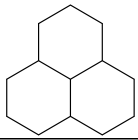
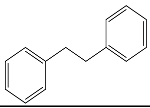
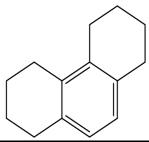
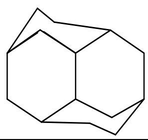
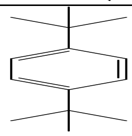
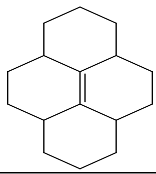
Table S2: The Table lists 111 identified organic species, including the protonated m/z, molecular formula, names of probable compounds, the structure of a potential contributor (many other structural possibilities may be feasible), LoD (Limit of detection) along with the average mixing ratios (ppb) observed during the monsoon (July-Sep 2022) and post-monsoon (Oct-Nov 2022) seasons. Also provided are each compound's Interquartile Range (IQR), and diel emission profile indicative of whether its ambient levels are driven by primary emissions, photochemical formation/ biogenic/ evaporative or both.

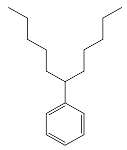
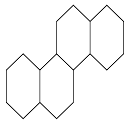
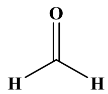
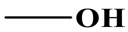
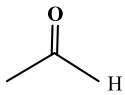
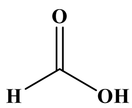
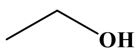
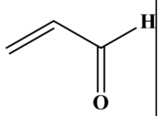
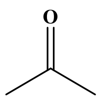
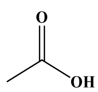
Sr No.	Type	Protonated m/z	Molecular formula	Major Potential contributors	Structure of a potential contributor	Average [Monsoon] (ppb) IQR	Average [post monsoon] (ppb) IQR	LoD (ppt)	Diurnal characteristics
1	Pure Hydrocarbon	41.035	**C_3H_4**	Propyne		3.043 (1.841)	9.997 (7.96)	37	Unimodal pattern with the evening peak
2		43.051	**C_3H_6**	Propene		1.88 (1.21)	4.965 (3.986)	11	Bimodal pattern with morning and evening peaks
3		53.035	**C_4H_4**	Vinylacetylene, 1-Buten-3-yne		0.081 (0.055)	0.722 (0.778)	15	Bimodal pattern with morning and evening peaks
4		55.051	**C_4H_6**	1,3-Butadiene, 1-Butyne, 2-Butyne, 1,2-Butadiene		1.067 (0.555)	2.78 (1.913)	22	Bimodal pattern with morning and

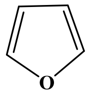
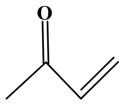
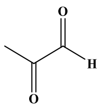
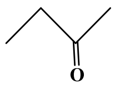
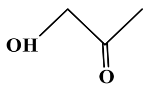
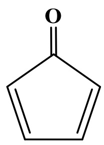
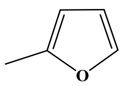
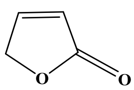
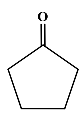
									evening peaks
5		57.067	**C_4H_8**	Methyl tert-butyl ether (MTBE) fragment / 1-Butene		1.813 (1.089)	5.578 (4.581)	21	Bimodal pattern with morning and evening peaks
6		67.051	**C_5H_6**	Cyclopentadiene, monoterpene fragment, butanol fragment		0.172 (0.108)	0.497 (0.336)	3	Bimodal pattern with afternoon and evening peaks
7		69.067	**C_5H_8**	Isoprene + 2-methyl-3-butene-2-ol fragment		0.667 (0.582)	1.118 (0.949)	6	Unimodal pattern with afternoon peak in monsoon while bimodal pattern with afternoon and evening peak in post-monsoon
8		79.052	**C_6H_6**	Benzene		0.802 (0.633)	3.724 (3.77)	3	Bimodal pattern with morning and evening peaks
9		83.084	**C_6H_{10}**	Cyclohexene, Hexyne isomers		0.319 (0.169)	0.624 (0.474)	5	Bimodal pattern with afternoon and evening peaks
10		85.099	**C_6H_{12}**	Cyclohexane, Hexene		0.058 (0.036)	0.16 (0.134)	2	Bimodal pattern with morning and evening peaks
11		91.053	**C_7H_6**	Monoterpene Fragment		0.102 (0.077)	0.714 (0.745)	2	Bimodal pattern with morning and evening peaks

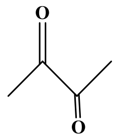
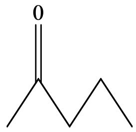
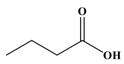
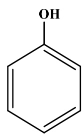
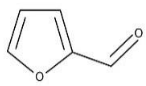
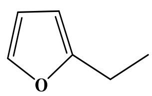
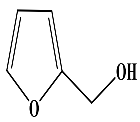
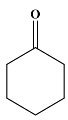
12		93.069	**C_7H_8**	Toluene		2.148 (1.813)	9.372 (10.377)	4	Bimodal pattern with morning and evening peaks
13		95.084	**C_7H_{10}**	Monoterpene Fragment		0.103 (0.057)	0.404 (0.293)	3	Bimodal pattern with morning and evening peaks
14		97.1	**C_7H_{12}**	Cycloheptene, Alkyl fragment		0.1 (0.058)	0.272 (0.217)	3	Bimodal pattern with afternoon and evening peaks
15		99.116	**C_7H_{14}**	Methylcyclohexane, Heptene & other hydrocarbons		0.005 (0.003)	0.014 (0.01)	1	Bimodal pattern with afternoon and evening peaks
16		105.069	**C_8H_8**	Styrene		0.167 (0.104)	0.699 (0.684)	1	Bimodal pattern with morning and evening peaks
17		107.085	**C_8H_{10}**	Sum of C8-Aromatics		1.123 (1.025)	5.017 (5.247)	1	Bimodal pattern with morning and evening peaks
18		109.1	**C_8H_{12}**	Terpene fragment/Cyclooctadiene		0.064 (0.032)	0.205 (0.174)	2	Bimodal pattern with afternoon and evening peaks
19		111.116	**C_8H_{14}**	Ethenyl cyclohexane		0.062 (0.035)	0.159 (0.137)	1	Bimodal pattern with afternoon and evening peaks
20		119.085	**C_9H_{10}**	Terpene fragment		0.063 (0.04)	0.233 (0.214)	0.4	Bimodal pattern with afternoon and evening peaks

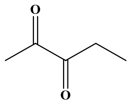
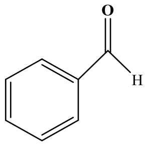
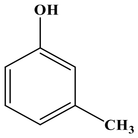
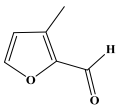
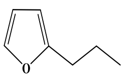
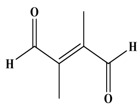
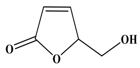
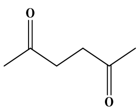
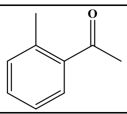
21		121.101	**C_9H_{12}**	Sum of C-9 aromatics		0.483 (0.449)	2.267 (2.323)	1	Bimodal pattern with morning and evening peaks
22		123.116	**C_9H_{14}**	Santene, 1,3-Cyclopentadiene & other hydrocarbons		0.039 (0.019)	0.123 (0.11)	1	Bimodal pattern with afternoon and evening peaks
23		125.133	**C_9H_{16}**	Nonyne, non-1,8-diene		0.021 (0.011)	0.049 (0.043)	1	Bimodal pattern with afternoon and evening peaks
24		129.07	**$C_{10}H_8$**	Naphthalene		0.09 (0.052)	0.381 (0.343)	1	Bimodal pattern with morning and evening peaks
25		133.102	**$C_{10}H_{12}$**	Ethyl styrene, tetrahydronaphthalene		0.044 (0.028)	0.154 (0.134)	0.5	Bimodal pattern with morning and evening peaks
26		135.118	**$C_{10}H_{14}$**	P-cymene, C4-substituted benzene, C2-substituted xylene		0.182 (0.153)	0.912 (0.87)	0.4	Bimodal pattern with morning and evening peaks
27		137.133	**$C_{10}H_{16}$**	Sum of Monoterpenes (MT)		0.172 (0.108)	0.497 (0.336)	1	Bimodal pattern with morning and evening peaks
28		143.086	**$C_{11}H_{10}$**	Methyl naphthalene		0.014 (0.009)	0.063 (0.059)	0.4	Bimodal pattern with morning and evening peaks
29		145.102	**$C_{11}H_{12}$**	C2 substituted indene		0.007 (0.004)	0.017 (0.016)	1	Trimodal pattern

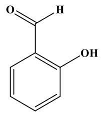
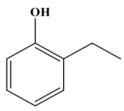
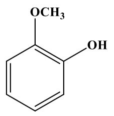
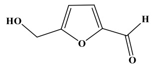
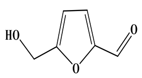
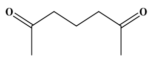
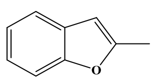
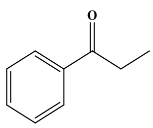
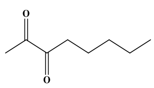
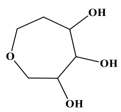
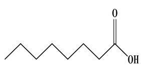
30		147.118	**$C_{11}H_{14}$**	Cyclopentylbenzene & other hydrocarbons		0.035 (0.022)	0.086 (0.079)	1	Trimodal pattern
31		157.099	**$C_{12}H_{12}$**	C2-substituted naphthalene		0.014 (0.006)	0.039 (0.032)	1	Bimodal pattern with afternoon and evening peaks
32		161.134	**$C_{12}H_{16}$**	Cyclohexylbenzene, butyl styrene, cyclopentylmethylbenzene		0.015 (0.009)	0.042 (0.038)	0.3	Trimodal pattern
33		175.15	**$C_{13}H_{18}$**	1,1,6-Trimethyltetralin/ ionene		0.006 (0.004)	0.022 (0.021)	0.3	Trimodal pattern
34		177.165	**$C_{13}H_{20}$**	C7-substituted benzene,		0.011 (0.006)	0.03 (0.028)	0.4	Trimodal pattern
35		179.181	**$C_{13}H_{22}$**	C3-substituted adamantane		0.004 (0.003)	0.015 (0.014)	0.4	Trimodal pattern
36		183.121	**$C_{14}H_{14}$**	Bibenzyl		0.003 (0.002)	0.006 (0.004)	0.4	Unimodal pattern with afternoon peak
37		187.148	**$C_{14}H_{18}$**	C4-substituted dihydroazulene, benzyl cycloheptene		0.004 (0.002)	0.008 (0.006)	0.3	Unimodal pattern with afternoon peak
38		189.165	**$C_{14}H_{20}$**	C4-substituted dihydronaphthalene, cyclopentylpropylbenzene		0.004 (0.003)	0.012 (0.011)	0.2	Trimodal pattern
39		191.181	**$C_{14}H_{22}$**	C8-substituted benzene		0.005 (0.004)	0.015 (0.014)	0.3	Trimodal pattern
40		217.195	**$C_{16}H_{24}$**	C6-substituted dihydronaphthalene		0.002 (0.001)	0.005 (0.004)	0.2	Trimodal pattern

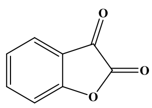
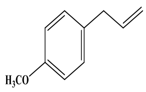
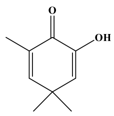
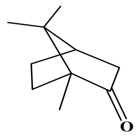
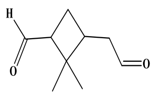
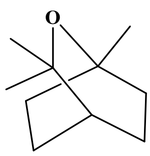
41		233.228	$\mathbf{C_{17}H_{28}}$	C11-substituted benzene		0.002 (0.001)	0.004 (0.003)	0.2	Bimodal pattern with afternoon and evening peaks
42		247.243	$\mathbf{C_{18}H_{30}}$	C12-substituted benzene		0.002 (0.002)	0.003 (0.002)	0.2	Unimodal pattern with afternoon peak
43	OXYGENATED VOCS	31.014	CH_2O	Formaldehyde		0.359 (0.233)	1.706 (1.249)	38	Bimodal pattern with afternoon and evening peaks
44		33.03	CH_4O	Methanol		9.854 (4.928)	19.919 (13.854)	25	Bimodal pattern with monsoon and evening peaks
45		45.03	$\mathbf{C_2H_4O}$	Acetaldehyde		3.339 (1.866)	7.755 (5.8)	21	Bimodal pattern with afternoon and evening peaks
46		47.009	$\mathbf{CH_2O_2}$	Formic acid		0.716 (0.568)	1.32 (1.096)	16	Unimodal pattern with afternoon peak
47		47.046	C_2H_6O	Ethanol		0.212 (0.16)	0.55 (0.505)	2	Bimodal pattern with morning and evening peaks
48		57.03	$\mathbf{C_3H_4O}$	Acrolein		0.157 (0.096)	0.674 (0.598)	6	Bimodal pattern with morning and evening peaks
49		59.046	$\mathbf{C_3H_6O}$	Acetone + Propanal		3.647 (2.162)	10.593 (8.485)	13	Bimodal pattern with afternoon and evening peaks
50		61.025	$\mathbf{C_2H_4O_2}$	Acetic acid+ Glycolaldehyde		4.103 (3.342)	6.585 (5.269)	9	Trimodal pattern

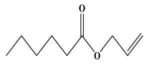
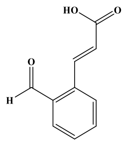
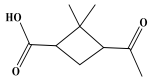
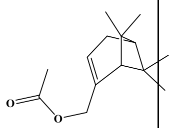
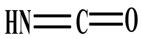
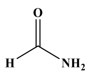
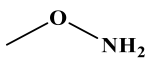
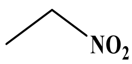
51		69.031	$\mathbf{C_4H_4O}$	Furan		0.032 (0.019)	0.168 (0.135)	1	Bimodal pattern with morning and evening peaks
52		71.047	$\mathbf{C_4H_6O}$	Methyl Vinyl Ketone, Methacrolein, 2-Butenal		0.291 (0.189)	0.498 (0.419)	4	Bimodal pattern with morning and evening peaks
53		73.026	$\mathbf{C_3H_4O_2}$	Methyl glyoxal		0.161 (0.109)	0.261 (0.259)	13	Unimodal pattern with afternoon peak
54		73.062	$\mathbf{C_4H_8O}$	Butanal, 2-Butanone, MEK		0.555 (0.388)	1.418 (1.195)	3	Bimodal pattern with morning and evening peaks
55		75.042	$\mathbf{C_3H_6O_2}$	Hydroxyacetone		0.278 (0.143)	1.012 (0.849)	3	Bimodal pattern with morning and evening peaks
56		81.031	$\mathbf{C_5H_4O}$	2,4-Cyclopentadiene-1-one		0.014 (0.007)	0.06 (0.055)	1	Bimodal pattern with morning and evening peaks
57		83.047	$\mathbf{C_5H_6O}$	2-Methyl furan		0.05 (0.026)	0.205 (0.157)	2	Bimodal pattern with morning and evening peaks
58		85.027	$\mathbf{C_4H_4O_2}$	2-Furanone / butenedial		0.05 (0.034)	0.275 (0.213)	2	Bimodal pattern with afternoon and evening peaks
59		85.063	$\mathbf{C_5H_8O}$	Cyclopentanone		0.06 (0.03)	0.167 (0.132)	1	Bimodal pattern with afternoon and evening peaks

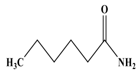
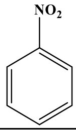
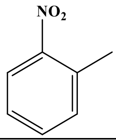
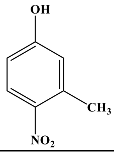
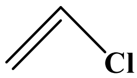
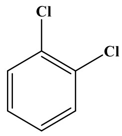
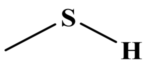
60		87.043	**$C_4H_6O_2$**	2,3 butanedione/ biacetyl		0.175 (0.094)	0.566 (0.465)	5	Bimodal pattern with afternoon and evening peaks
61		87.079	**$C_5H_{10}O$**	2-Pentanone, 2-methyl-3-butene-2-ol, Pentanal		0.052 (0.031)	0.141 (0.132)	1	Bimodal pattern with afternoon and evening peaks
62		89.058	**$C_4H_8O_2$**	Butanoic acid, Ethyl acetate		0.281 (0.234)	0.533 (0.449)	2	Bimodal pattern with morning and afternoon peaks
63		95.048	**C_6H_6O**	Phenol		0.097 (0.057)	0.418 (0.352)	3	Trimodal pattern in monsoon while bimodal pattern with morning and evening peaks in post-monsoon
64		97.027	**$C_5H_4O_2$**	Furfural		0.048 (0.036)	0.355 (0.294)	2	Bimodal pattern with morning and evening peaks
65		97.063	**C_6H_8O**	C2 substituted furan, 2-methyl-2-Cyclopenten-1-one		0.034 (0.016)	0.132 (0.098)	2	Bimodal pattern with morning and evening peaks
66		99.043	**$C_5H_6O_2$**	Furfuryl alcohol, 3-Methyl-2-furanone, 4-Methyl-5H-furan-2-one		0.081 (0.059)	0.267 (0.251)	3	Unimodal pattern with afternoon peak
67		99.079	**$C_6H_{10}O$**	Cyclohexanon e		0.167 (0.109)	0.424 (0.346)	2	Bimodal pattern with afternoon and evening peaks

68		101.059	**$C_5H_8O_2$**	2,3-Pentanedione, methyl methacrylate & other hydrocarbons		0.129 (0.074)	0.304 (0.268)	2	Bimodal pattern with afternoon and evening peaks
69		107.049	**C_7H_6O**	Benzaldehyde		0.06 (0.046)	0.202 (0.19)	1	Bimodal pattern with afternoon and evening peaks
70		109.064	**C_7H_8O**	Methylphenol isomers, Anisole		0.027 (0.016)	0.1 (0.078)	1	Bimodal pattern with morning and evening peaks
71		111.042	**$C_6H_6O_2$**	5-Methylfurfural, Hydroxyphenol		0.015 (0.01)	0.097 (0.083)	2	Trimodal pattern in monsoon while Bimodal pattern with morning and evening peak in post-monsoon
72		111.08	**$C_7H_{10}O$**	C3-substituted furans, C2-substituted cyclopentene, methyl cyclohexene		0.021 (0.011)	0.081 (0.068)	1	Bimodal pattern with morning and evening peaks
73		113.059	**$C_6H_8O_2$**	Dimethylbutenedial / C4-substituted aldehydeyde		0.047 (0.027)	0.159 (0.159)	2	Bimodal pattern with morning and evening peaks
74		115.039	**$C_5H_6O_3$**	5-Hydroxymethyl-2-furanone/ methylepoxybutanedial		0.014 (0.01)	0.046 (0.046)	1	Unimodal pattern with afternoon peak
75		115.075	**$C_6H_{10}O_2$**	C6 diketone isomers/ C6 esters		0.051 (0.028)	0.124 (0.121)	2	Unimodal pattern with afternoon peak
76		121.064	**C_8H_8O**	Tolualdehyde		0.065 (0.046)	0.209 (0.195)	1	Bimodal pattern with afternoon

									and evening peaks
77		123.044	**$C_7H_6O_2$**	2-Hydroxybenzaldehyde		0.027 (0.017)	0.119 (0.104)	1	Unimodal pattern with afternoon peak
78		123.08	**$C_8H_{10}O$**	C2-substituted phenol, methyl anisole		0.015 (0.008)	0.054 (0.046)	1	Bimodal pattern with morning and evening peaks
79		125.06	**$C_7H_8O_2$**	Guaiacol		0.016 (0.009)	0.06 (0.049)	1	Bimodal pattern with afternoon and evening peaks
80		127.039	**$C_6H_6O_3$**	Hydroxymethyl furfural		0.009 (0.006)	0.044 (0.039)	2	Unimodal pattern with afternoon peak
81		127.075	**$C_7H_{10}O_2$**	Trimethylbutenedial / Methyl sorbate		0.025 (0.013)	0.077 (0.07)	1	Unimodal pattern with afternoon peak
82		129.092	**$C_7H_{12}O_2$**	C7-diketone/heptane-2,6-dione		0.025 (0.016)	0.051 (0.049)	1	Unimodal pattern with afternoon peak
83		133.065	**C_9H_8O**	Methyl benzofuran		0.007 (0.003)	0.027 (0.023)	0.3	Bimodal pattern with morning and evening peaks
84		135.08	**$C_9H_{10}O$**	3-Methylacetophenone		0.016 (0.01)	0.058 (0.054)	0.4	Bimodal pattern with morning and evening peaks
85		143.108	**$C_8H_{14}O_2$**	2,3-Octanedione		0.02 (0.011)	0.04 (0.035)	1	Unimodal pattern with afternoon peak
86		145.051	**$C_6H_8O_4$**	Organic acids/ levoglucosan fragment		0.006 (0.003)	0.022 (0.018)	1	Unimodal pattern with afternoon peak
87		145.123	**$C_8H_{16}O_2$**	n-Octanoic acid		0.030 (0.017)	0.059 (0.048)	1	Unimodal pattern with afternoon

									peak in monsoon while bimodal pattern with afternoon and evening peak in post-monsoon
88		149.024	**$C_8H_4O_3$**	Phthalic anhydride/ 2,3-Benzofurandione		0.014 (0.011)	0.062 (0.059)	2	Unimodal pattern with afternoon peak
89		149.096	**$C_{10}H_{12}O$**	Methyl chavicol (estragole)		0.007 (0.004)	0.03 (0.027)	1	Bimodal pattern with morning and evening peaks
90		153.092	**$C_9H_{12}O_2$**	Oxonopinone		0.009 (0.004)	0.029 (0.026)	1	Bimodal pattern with afternoon and evening peaks
91		153.128	**$C_{10}H_{16}O$**	Camphor, pinene oxide		0.022 (0.015)	0.096 (0.086)	1	Bimodal pattern with afternoon and evening peaks
92		155.108	**$C_9H_{14}O_2$**	Norpinonaldehyde		0.012 (0.006)	0.026 (0.022)	1	Unimodal pattern with afternoon peak
93		155.144	**$C_{10}H_{18}O$**	Cineole, Linalool, 4-tert-butyl cyclohexanone		0.01 (0.007)	0.023 (0.019)	1	Unimodal pattern with afternoon peak in monsoon while bimodal pattern with afternoon and evening peak in post-monsoon

94		157.122	**$C_9H_{16}O_2$**	C9- ester		0.013 (0.007)	0.026 (0.023)	1	Unimodal pattern with afternoon peak
95		159.14	**$C_9H_{18}O_2$**	C9-organic acid		0.020 (0.012)	0.038 (0.031)	1	Unimodal pattern with afternoon peak
96		177.056	**$C_{10}H_8O_3$**	2-Formylcinnamic acid / hydroxy-methyl-coumarin		0.008 (0.005)	0.026 (0.022)	1	Bimodal pattern with afternoon and evening peaks
97		185.121	**$C_{10}H_{16}O_3$**	cis-Pinonic acid		0.006 (0.004)	0.01 (0.008)	0.4	Unimodal pattern with afternoon peak
98		195.138	**$C_{12}H_{18}O_2$**	Myrtenyl acetate		0.002 (0.001)	0.006 (0.006)	0.4	Unimodal pattern with afternoon peak
99		42.03	C_2H_3N	Acetonitrile		0.291 (0.126)	0.942 (0.714)	4	Bimodal pattern with morning and evening peaks
100		44.018	HNCO	Isocyanic acid		0.051 (0.038)	0.139 (0.095)	4	Bimodal pattern with morning and afternoon peaks
101	NVOCS	46.025	CH_3NO	Formamide		0.232 (0.206)	0.296 (0.236)	6	Unimodal pattern with afternoon peak
102		48.048	CH_5NO	methoxyamine		0.003 (0.002)	0.01 (0.009)	1	Bimodal pattern with morning and evening peaks
103		76.037	**$C_2H_5NO_2$**	Nitroethane		0.009 (0.005)	0.213 (0.206)	0.5	Unimodal pattern with afternoon peak
104		84.08	**C_5H_9N**	Pentanenitrile/ Methylbutanenitrile isomers/ C5-amines		0.005 (0.003)	0.021 (0.022)	0.5	Bimodal pattern with morning and

									evening peaks
105		116.108	**$C_6H_{13}NO$**	C6-amide		0.006 (0.004)	0.01 (0.007)	0.2	Unimodal pattern with afternoon peak
106		124.039	**$C_6H_5NO_2$**	Nitrobenzene		0.006 (0.004)	0.019 (0.018)	1	Trimodal pattern
107		138.056	**$C_7H_7NO_2$**	Nitrotoluene/ salicylamide		0.003 (0.001)	0.013 (0.01)	0.5	Trimodal pattern
108		154.052	**$C_7H_7NO_3$**	Nitrobenzyl alcohol/Nitrocresols, methyl-nitrophenol		0.005 (0.004)	0.024 (0.025)	0.5	Trimodal pattern
109	ClVOCS	62.997	**C_2H_3Cl**	Vinyl chloride		0.004 (0.003)	0.015 (0.011)	1	Bimodal pattern with afternoon and evening peaks
110		146.977	**$C_6H_4Cl_2$**	Dichlorobenzene		0.025 (0.021)	0.115 (0.121)	0.1	Bimodal pattern with morning and evening peaks
111	SVOCS	49.007	**CH_4S**	Methanethiol		0.048 (0.047)	0.128 (0.129)	1	Bimodal pattern with morning and evening peaks

- Bold ones in Molecular formula column are those compounds whose isotopic peaks were observed

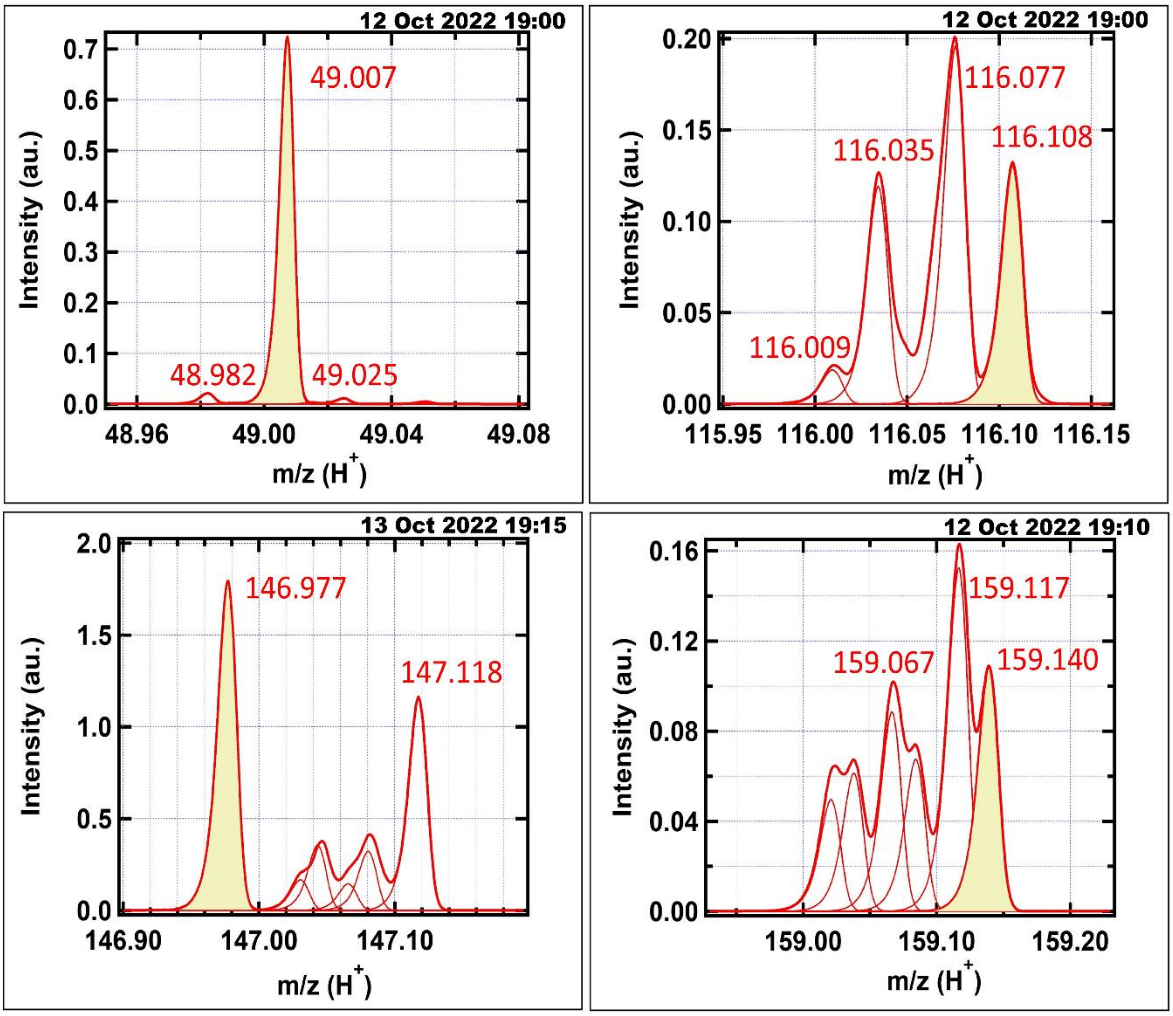


Figure S1 Example of mass spectra and peak assignment using IDA software which also illustrate the high mass resolving power of the PTR-ToF-MS 10K enabling separation of ion signals that land at the same nominal masses.

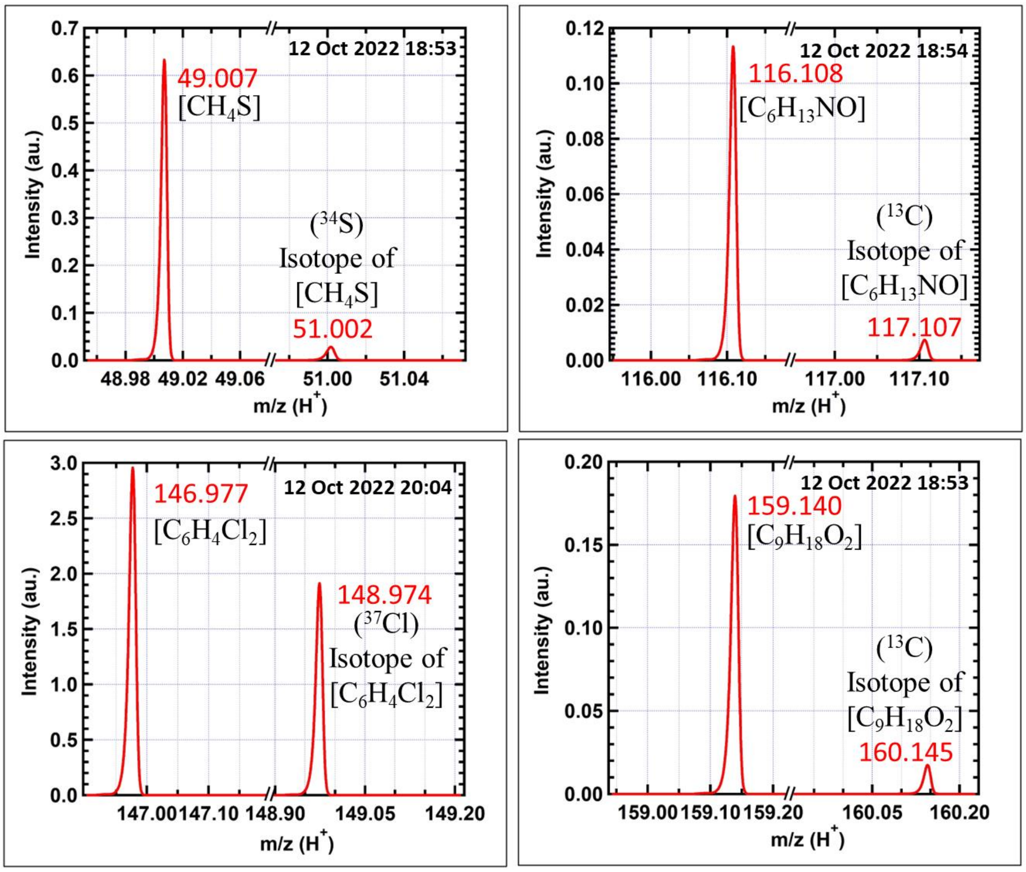


Figure S2 Mass spectra of methanethiol, dichlorobenzene, C6-amide and C9- carboxylic acid which also illustrate the high mass resolving power of the PTR-ToF-MS 10K enabling identification of isotopic peaks

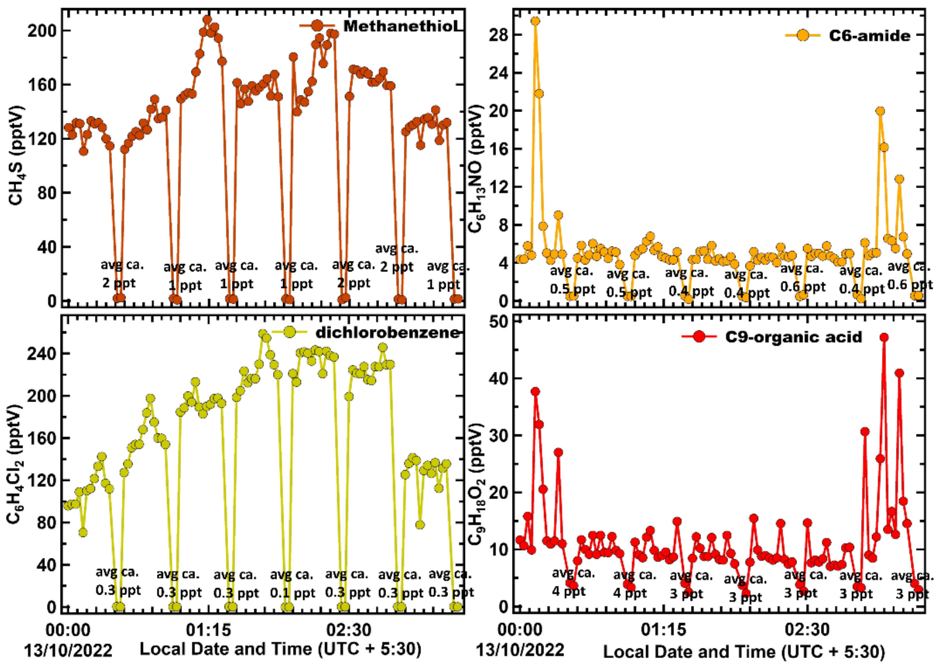


Figure S3: Example of measured data showing the ambient data and instrument background mixing ratios (2 min avg) for methanethiol, dichlorobenzene, C-6 amide and C-9 carboxylic acid.

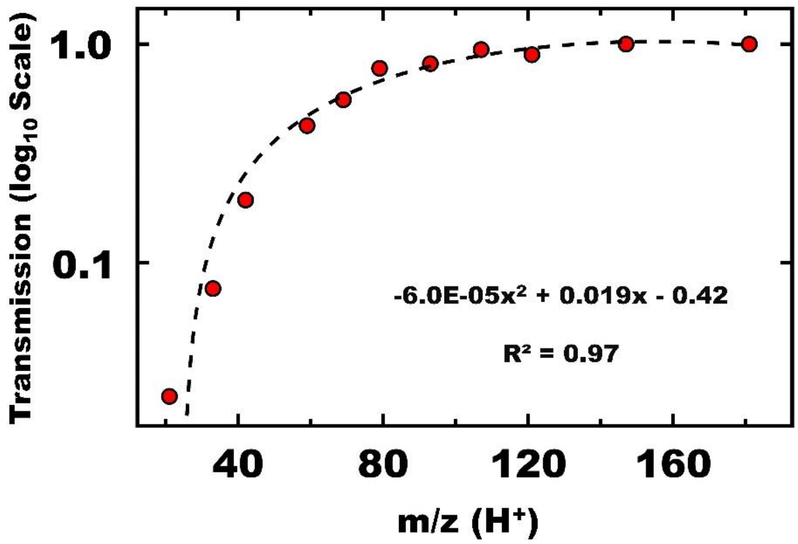


Figure S4: Transmission values as a function of m/z for the PTR-TOF-MS 10K obtained during a calibration experiment performed on 26th September 2022 using the VOC calibration gas mixture (Societa Italiana Acetilene E Derviati; S.I.A.D. S.p.A., Italy) containing 11 hydrocarbons at ~100 ppb, namely methanol, acetonitrile, acetone, isoprene, benzene, toluene, xylene, trimethylbenzene, and dichlorobenzene and trichlorobenzene

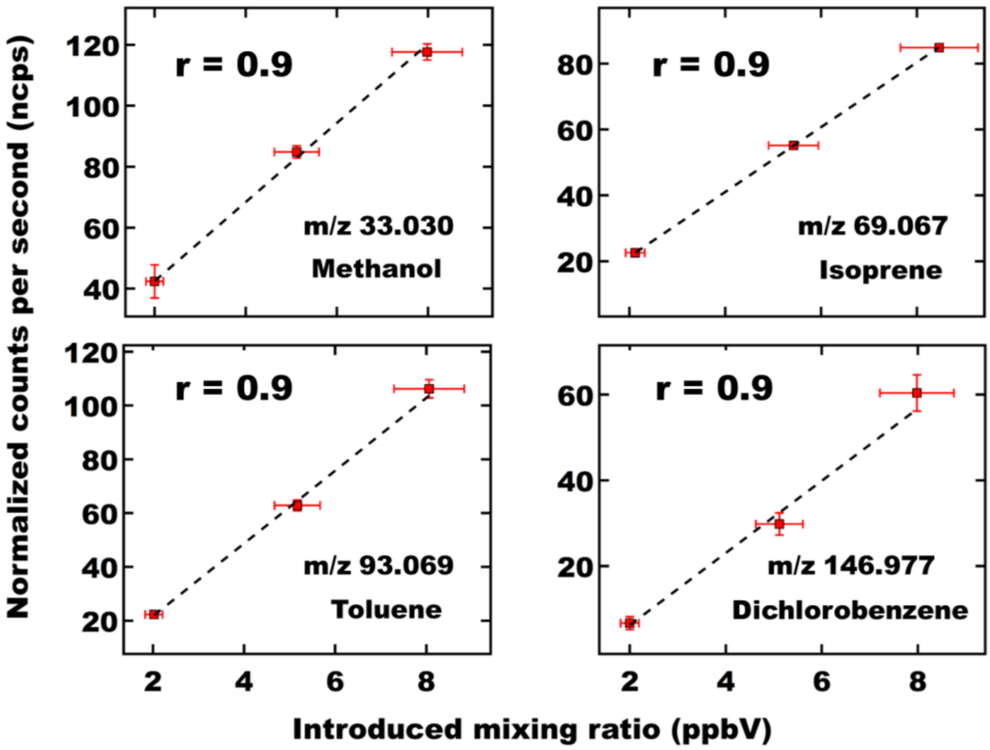


Figure S5 Sensitivity (ncps/ppb) and linearity of selected VOCs in the calibration experiment (PTR-MS) performed on 26/09/2022. The horizontal error bars represent the root mean square propagation of errors due to 10% uncertainty in the VOC standard and 2% error for each of the two mass flow controllers used for calibration. The vertical error bars represent the standard deviation (σ) instrumental precision error while sampling the standard gas at each dilution mixing ratio.

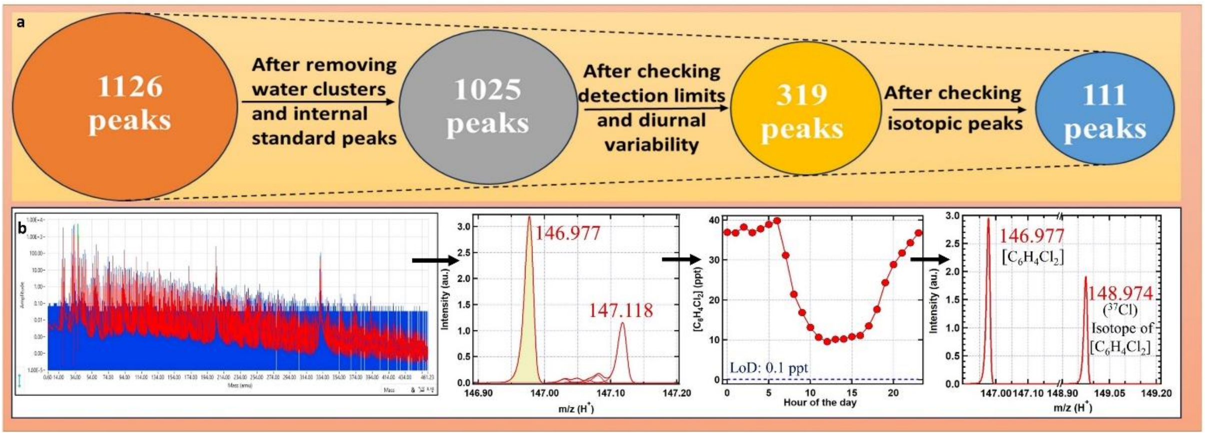


Figure S6 Visual representation of the process providing also an example compound attribution to an ion (for m/z 146.977; dichlorobenzene) showing isotopic peak match with theoretically predicted isotopic abundance

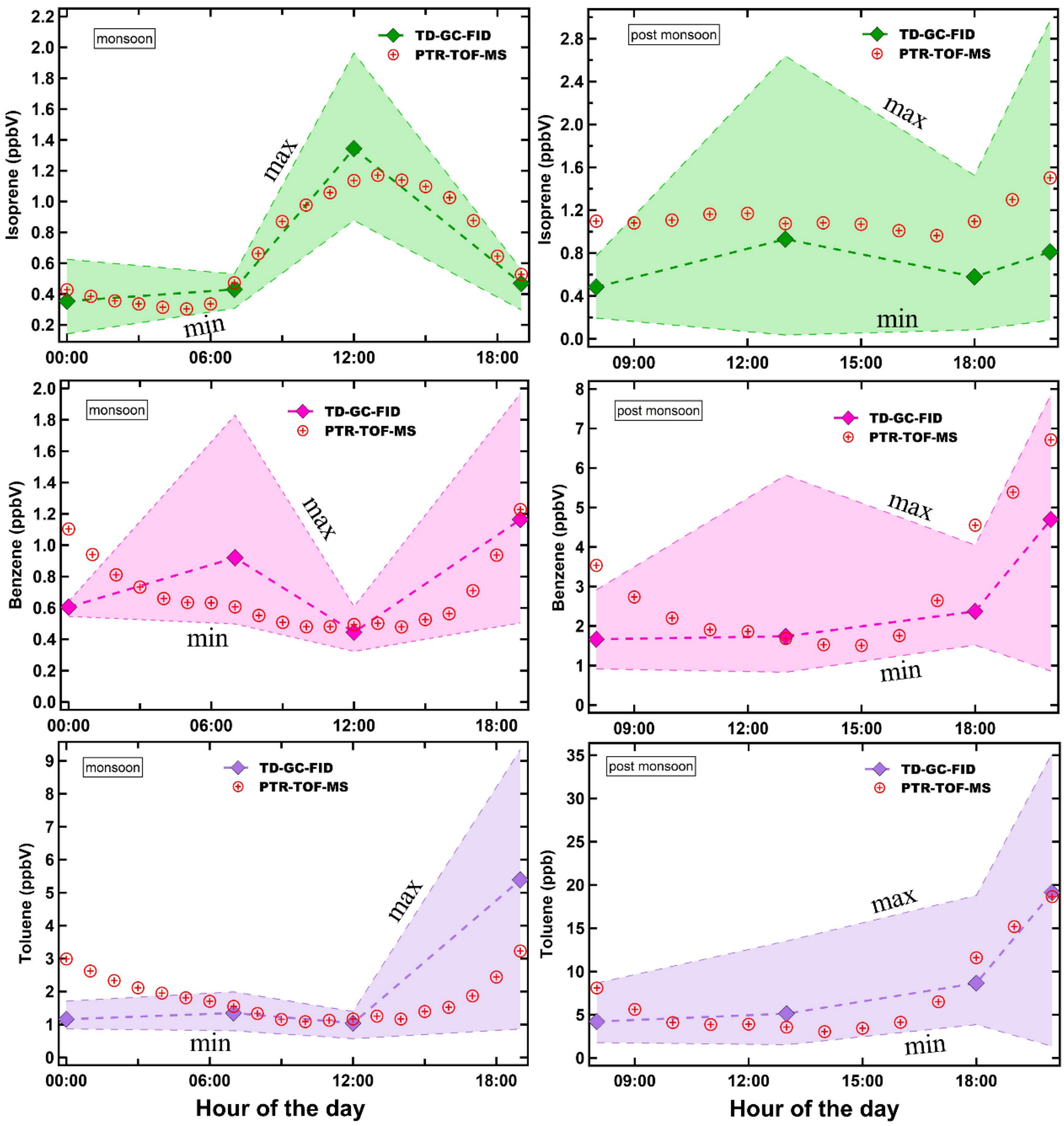


Figure S7: Season-wise hourly averaged average mixing ratios of isoprene, benzene and toluene measured using the TD-GC-FID are shown as diamonds and minimum and maximum values for that hourly sampling interval as shaded regions (in green for isoprene, pink for benzene and purple for toluene). The PTR-TOF-MS season-average mixing ratios values presented in Figure 4 are also shown for reference (red circles). During the campaign whole air samples were collected into 6 L passivated SilcoCan air sampling steel canisters (Restek) (Kumar et al., 2020; Vettikkat et al., 2020, Shabin et al., 2024) from the rooftop of the same building to measure isoprene, toluene and benzene using a thermal desorption gas chromatograph coupled to a flame ionisation detector (TD-GC-FID). Technical details pertaining to the TD-GC-FID measurements are available in Shabin et al., 2024. Air samples were collected near the PTR-TOF-MS inlet on the rooftop during post monsoon season, four times a day [during hourly intervals corresponding to 08:00, 13:00, 18:00, 20:00 local time (n=39,) and during monsoon season also four times a day during hourly intervals corresponding to: 00:00, 07:00, 12:00, 19:00 local time (n=15).

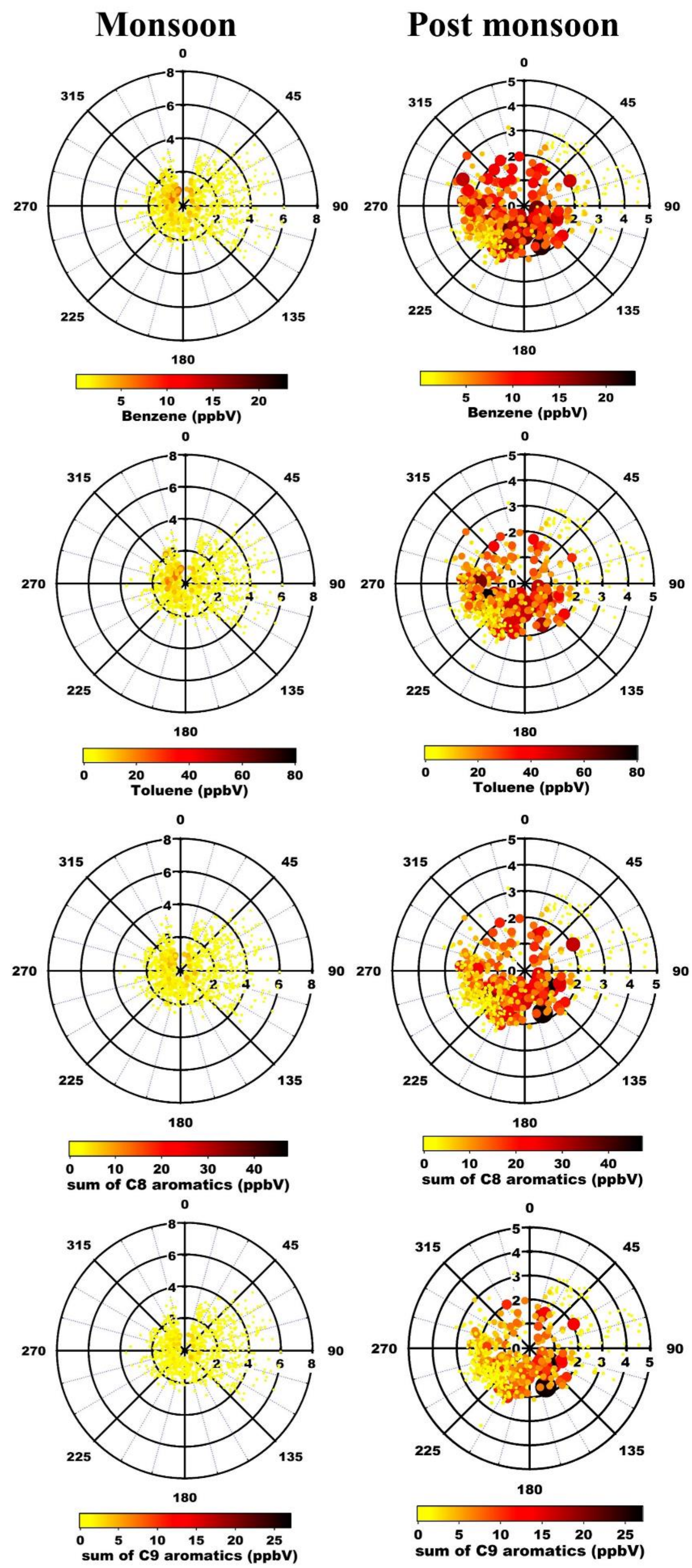


Figure S8 Wind rose of night-time benzene, toluene, C8 and C9 aromatic compounds at the receptor site during monsoon (left column) and post monsoon (right column) season

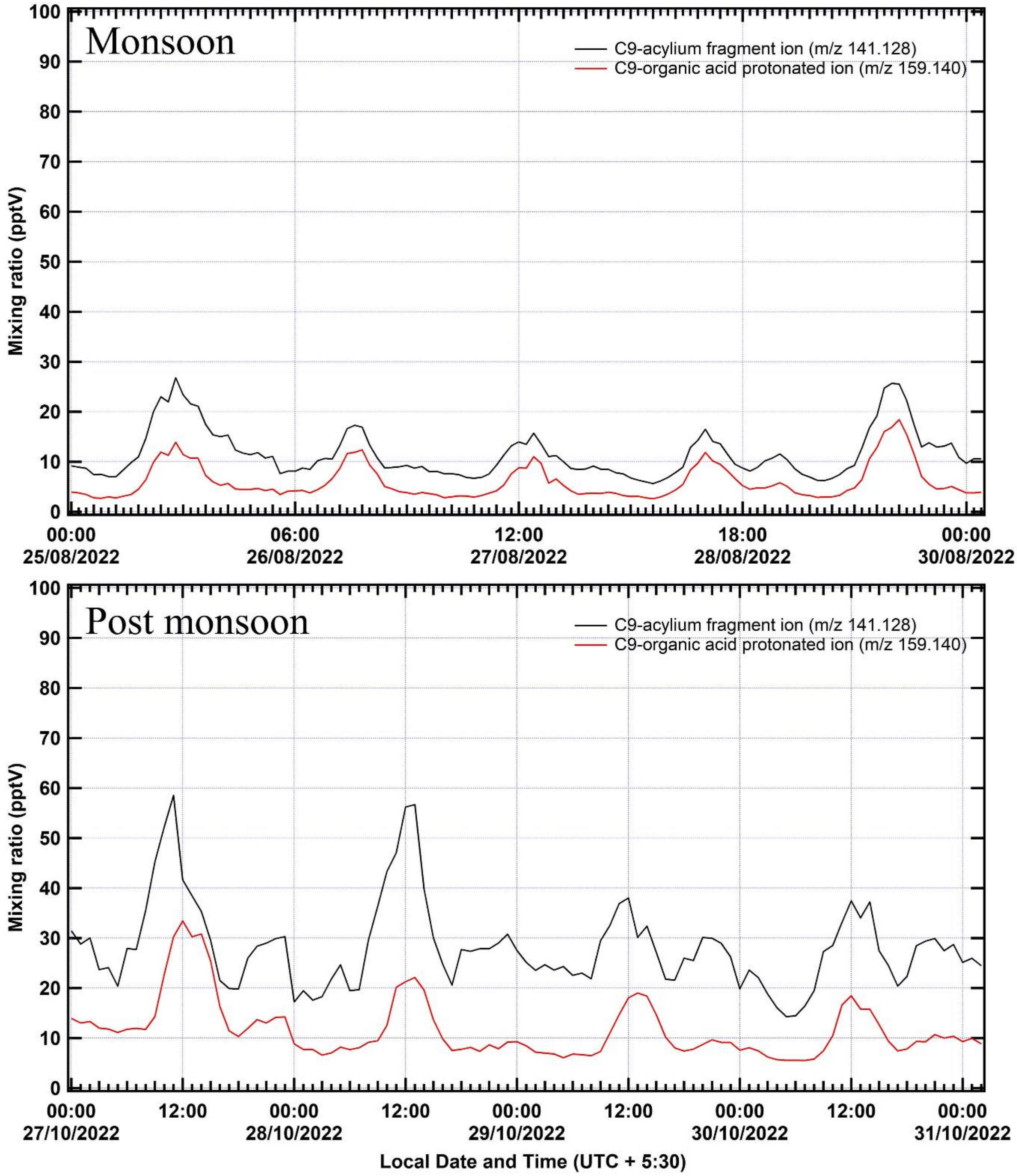


Figure S9: Time series of C9-acylium fragmentation ion and C9-organic acid protonated ion during monsoon (25th Aug 2022 to 30th Aug 2022) and post monsoon season (27th Oct 2022 to 31st Oct 2022) provided for illustration

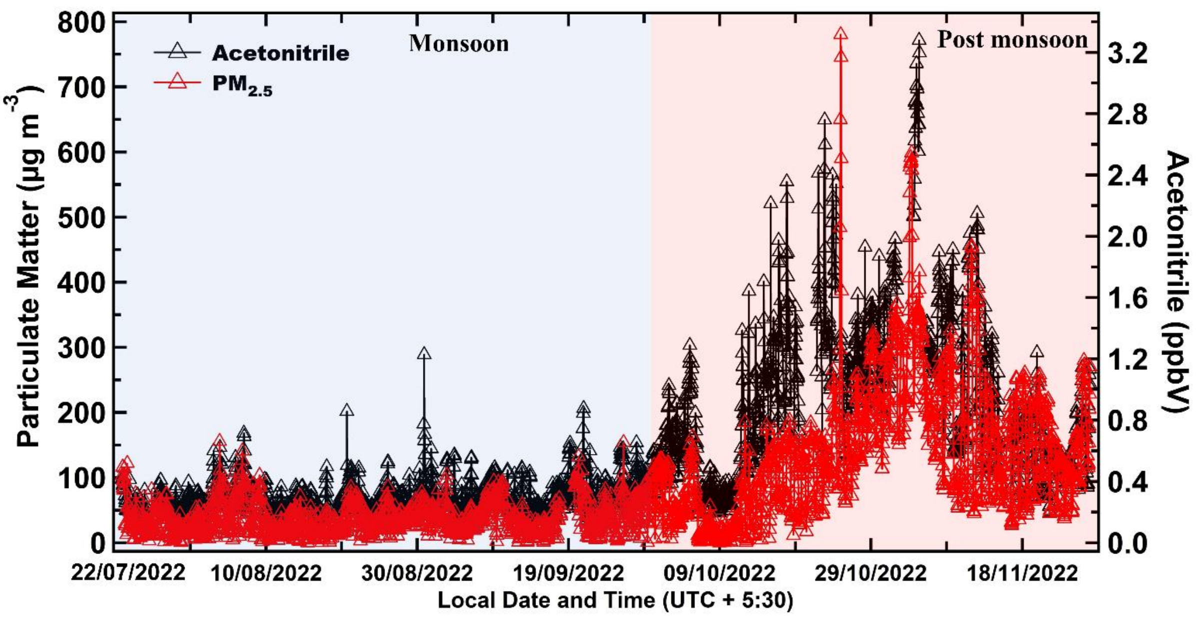


Figure S10: Time series of hourly $PM_{2.5}$ and acetonitrile measured at IMD Delhi site

$$[R]_{ppb} = 10^9 \times \frac{\mu_0 U_{drift}}{L^2 k_{VOC+H_3O^+}} \times \frac{P_0{}^2}{P_{drift}{}^2} \times \frac{T_{drift}{}^2}{T_0{}^2} \times \frac{22400}{N_A} \times \frac{I_{(RH^+)}}{I_{(H_3O^+)}} \times \frac{T_{H3O^+}}{T_{VOCH^+}} \quad \textbf{Equation S1}$$

Where $k_{VOC+H_3O^+}$= Rate constant of proton transfer from hydronium ion to a VOC

L = Length of drift tube (9.2 cm)

μ_o= Reduced mobility of H_3O^+ ions (2.8 cm^2 V^{-1} s^{-1})

N = Number density of gases in the drift tube

E= Electric field across the drift tube

U_{drift} = Voltage across the drift tube

P_{drift} & T_{drift} = Drift tube pressure and temperature

P_0 & T_0 = Standard pressure and temperature; N_A = Avogadro Number

$\frac{T_{VOCH^+}}{T_{H_3O^+}}$ = Ratio of transmission efficiency of protonated VOC ions and hydronium ions

Reference:

Shabin, M., Khatarkar, P., Hakkim, H, et al., Monsoon and post-monsoon measurements of 53 non-methane hydrocarbons (NMHCs) in megacity Delhi and Mohali reveal similar NMHC composition across seasons, Urban Climate, Volume 55, 101983, 2024.