

Discovery of reactive chlorine, sulphur and nitrogen containing ambient volatile organic compounds in the megacity of Delhi during both clean and extremely polluted seasons

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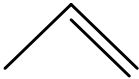



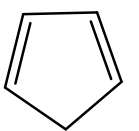
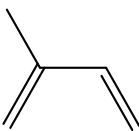
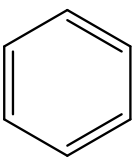
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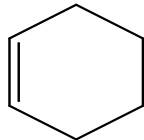

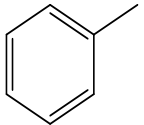
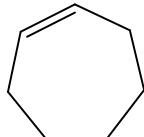
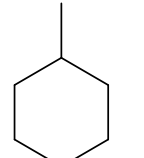
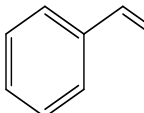
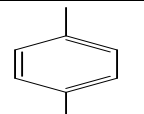
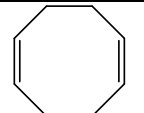
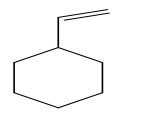
Table S1: Operational settings for PTR-TOF-MS 10 K parameters used during this deployment

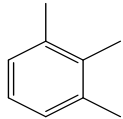
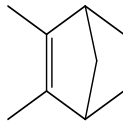

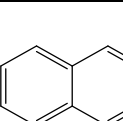
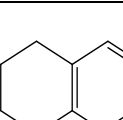
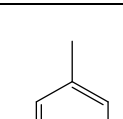
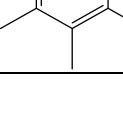
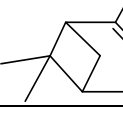
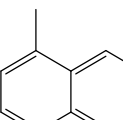
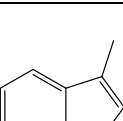
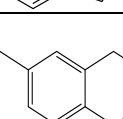
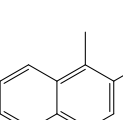
Parameters	Values
Overall drift voltage (U_{drift})	600 V
Temperature at drift tube (T_{drift})	120 °C
Pressure at drift tube (P_{drift})	3.0 mbar
Length of the drift tube (L_{drift})	9.2 cm
Extraction time (t)	26 μ s
Field strength of the drift tube (E/N)	120 Td

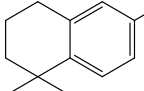
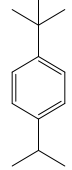
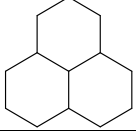
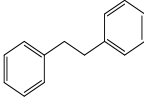
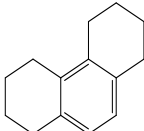
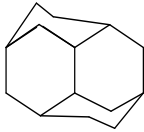
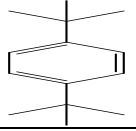
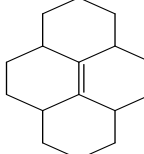
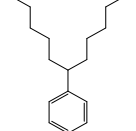
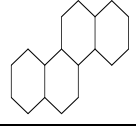
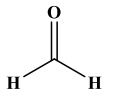
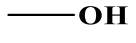
* E is the electric field strength (V cm^{-1}) and N is the gas number density (molecule cm^{-3}). $1 \text{ Td} = 10^{-17} \text{ V cm}^2 \text{ molecule}^{-1}$

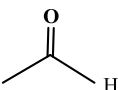
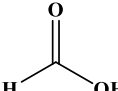
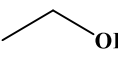
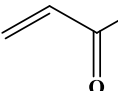
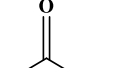
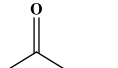
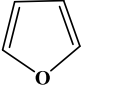
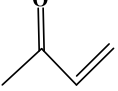
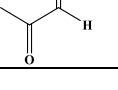
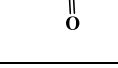
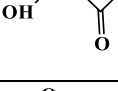
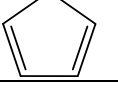
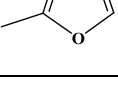
Table S2: The table lists 111 identified organic species, including the protonated m/z, molecular formula, names of probable compounds, the structure of a potential contributor (many others structural possibilities maybe feasible), along with the average mixing ratios (ppb) observed during the monsoon (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.

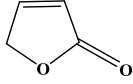
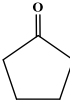
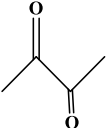
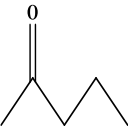
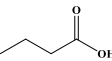
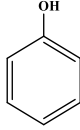
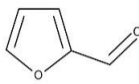
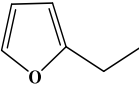
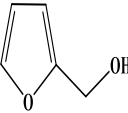
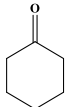
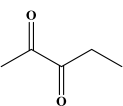
Sr No.	Type	Protonated m/z	Molecular formula	Major Potential contributors	Structure of a potential contributor	Average [Monsoon] (ppb) IQR	Average [post-monsoon] (ppb) IQR	Diurnal characteristics
1	Pure Hydrocarbon	41.035	C₃H₄	Propyne		3.043 (1.841)	9.997 (7.96)	Unimodal pattern with the evening peak
2		43.051	C₃H₆	Propene		1.88 (1.21)	4.965 (3.986)	Bimodal pattern with morning and evening peaks
3		53.035	C₄H₄	Vinylacetylene, 1-Buten-3-yne		0.081 (0.055)	0.722 (0.778)	Bimodal pattern with morning and evening peaks
4		55.051	C₄H₆	1,2-Butadiene, 1-Butyne, 2-Butyne 1,3 Butadiene		1.067 (0.555)	2.78 (1.913)	Bimodal pattern with morning and evening peaks
5		57.067	C₄H₈	Methyl tert-butyl ether (MTBE) fragment / 1-Butene		1.813 (1.089)	5.578 (4.581)	Bimodal pattern with morning and evening peaks
6		67.051	C₅H₆	Cyclopentadiene, monoterpene fragment, butanol fragment		0.172 (0.108)	0.497 (0.336)	Bimodal pattern with afternoon and evening peaks
7		69.067	C₅H₈	Isoprene + 2-methyl-3-butene-2-ol fragment		0.667 (0.582)	1.118 (0.949)	Unimodal pattern with afternoon peak in monsoon while bimodal pattern with afternoon and evening peak in post-monsoon
8		79.052	C₆H₆	Benzene		0.802 (0.633)	3.724 (3.77)	Bimodal pattern with morning and evening peaks

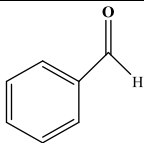
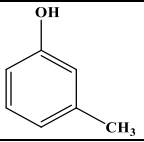
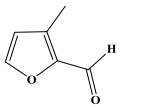
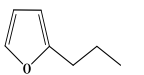
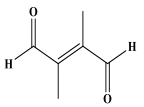
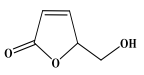
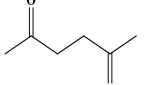
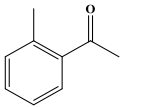
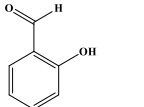
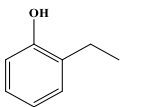
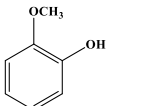
9	83.084	C₆H₁₀	Cyclohexene, Hexyne isomers		0.319 (0.169)	0.624 (0.474)	Bimodal pattern with afternoon and evening peaks
10	85.099	C₆H₁₂	Cyclohexane, Hexene		0.058 (0.036)	0.16 (0.134)	Bimodal pattern with morning and evening peaks
11	91.053	C₇H₆	Monoterpene Fragment		0.102 (0.077)	0.714 (0.745)	Bimodal pattern with morning and evening peaks
12	93.069	C₇H₈	Toluene		2.148 (1.813)	9.372 (10.377)	Bimodal pattern with morning and evening peaks
13	95.084	C₇H₁₀	Monoterpene Fragment		0.103 (0.057)	0.404 (0.293)	Bimodal pattern with morning and evening peaks
14	97.1	C₇H₁₂	Cycloheptene, Alkyl fragment		0.1 (0.058)	0.272 (0.217)	Bimodal pattern with afternoon and evening peaks
15	99.116	C₇H₁₄	Methylcyclohe xane, Heptene & other hydrocarbons		0.005 (0.003)	0.014 (0.01)	Bimodal pattern with afternoon and evening peaks
16	105.069	C₈H₈	Styrene		0.167 (0.104)	0.699 (0.684)	Bimodal pattern with morning and evening peaks
17	107.085	C₈H₁₀	Sum of C8- Aromatics		1.123 (1.025)	5.017 (5.247)	Bimodal pattern with morning and evening peaks
18	109.1	C₈H₁₂	Terpene fragment/Cyclo octadiene		0.064 (0.032)	0.205 (0.174)	Bimodal pattern with afternoon and evening peaks
19	111.116	C₈H₁₄	Ethenyl cyclohexane		0.062 (0.035)	0.159 (0.137)	Bimodal pattern with afternoon and evening peaks
20	119.085	C₉H₁₀	Terpene fragment		0.063 (0.04)	0.233 (0.214)	Bimodal pattern with afternoon and evening peaks

21	121.101	C₉H₁₂	Sum of C-9 aromatics		0.483 (0.449)	2.267 (2.323)	Bimodal pattern with morning and evening peaks
22	123.116	C₉H₁₄	Santene, 1,3-Cyclopentadiene & other hydrocarbons		0.039 (0.019)	0.123 (0.11)	Bimodal pattern with afternoon and evening peaks
23	125.133	C₉H₁₆	Nonyne, non-1,8-diene		0.021 (0.011)	0.049 (0.043)	Bimodal pattern with afternoon and evening peaks
24	129.07	C₁₀H₈	Naphthalene		0.09 (0.052)	0.381 (0.343)	Bimodal pattern with morning and evening peaks
25	133.102	C₁₀H₁₂	Ethyl styrene, tetrahydronaphthalene		0.044 (0.028)	0.154 (0.134)	Bimodal pattern with morning and evening peaks
26	135.118	C₁₀H₁₄	P-cymene, C4-substituted benzene, C2-substituted xylene		0.182 (0.153)	0.912 (0.87)	Bimodal pattern with morning and evening peaks
27	137.133	C₁₀H₁₆	Sum of Monoterpenes (MT)		0.172 (0.108)	0.497 (0.336)	Bimodal pattern with morning and evening peaks
28	143.086	C₁₁H₁₀	Methyl naphthalene		0.014 (0.009)	0.063 (0.059)	Bimodal pattern with morning and evening peaks
29	145.102	C₁₁H₁₂	C2 substituted indene		0.007 (0.004)	0.017 (0.016)	Trimodal pattern
30	147.118	C₁₁H₁₄	Cyclopentylbenzene & other hydrocarbons		0.035 (0.022)	0.086 (0.079)	Trimodal pattern
31	157.099	C₁₂H₁₂	C2-substituted naphthalene		0.014 (0.006)	0.039 (0.032)	Bimodal pattern with afternoon and evening peaks
32	161.134	C₁₂H₁₆	Cyclohexylbenzene, butyl styrene, cyclopentylmethylbenzene		0.015 (0.009)	0.042 (0.038)	Trimodal pattern

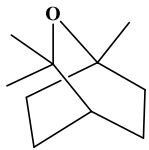
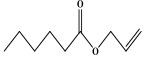

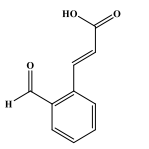

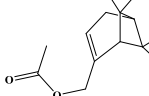

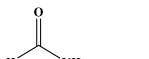
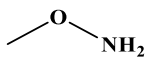
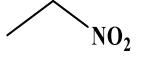

33		175.15	C₁₃H₁₈	1,1,6-Trimethyltetralin/ ionene		0.006 (0.004)	0.022 (0.021)	Trimodal pattern
34		177.165	C₁₃H₂₀	C7-substituted benzene,		0.011 (0.006)	0.03 (0.028)	Trimodal pattern
35		179.181	C₁₃H₂₂	C3-substituted adamantane		0.004 (0.003)	0.015 (0.014)	Trimodal pattern
36		183.121	C₁₄H₁₄	Bibenzyl		0.003 (0.002)	0.006 (0.004)	Unimodal pattern with afternoon peak
37		187.148	C₁₄H₁₈	C4-substituted dihydroazulene, benzyl cycloheptene		0.004 (0.002)	0.008 (0.006)	Unimodal pattern with afternoon peak
38		189.165	C₁₄H₂₀	C4-substituted dihydronaphthalene, cyclopentylpropylbenzene		0.004 (0.003)	0.012 (0.011)	Trimodal pattern
39		191.181	C₁₄H₂₂	C8-substituted benzene		0.005 (0.004)	0.015 (0.014)	Trimodal pattern
40		217.195	C₁₆H₂₄	C6-substituted dihydronaphthalene		0.002 (0.001)	0.005 (0.004)	Trimodal pattern
41		233.228	C₁₇H₂₈	C11-substituted benzene		0.002 (0.001)	0.004 (0.003)	Bimodal pattern with afternoon and evening peaks
42		247.243	C₁₈H₃₀	C12-substituted benzene		0.002 (0.002)	0.003 (0.002)	Unimodal pattern with afternoon peak
43	OXYGENATED VOCS	31.014	CH ₂ O	Formaldehyde		0.359 (0.233)	1.706 (1.247)	Bimodal pattern with afternoon and evening peaks
44		33.03	CH ₄ O	Methanol		9.854 (4.928)	19.919 (13.845)	Bimodal pattern with monsoon

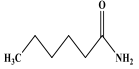
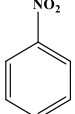
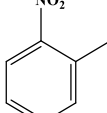
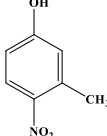
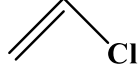
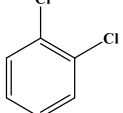
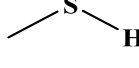
								and evening peaks
45	45.03	C₂H₄O	Acetaldehyde		3.339 (1.866)	7.755 (5.799)		Bimodal pattern with afternoon and evening peaks
46	47.009	CH₂O₂	Formic acid		0.716 (0.568)	1.32 (1.095)		Unimodal pattern with afternoon peak
47	47.046	C₂H₆O	Ethanol		0.212 (0.16)	0.55 (0.505)		Bimodal pattern with morning and evening peaks
48	57.03	C₃H₄O	Acrolein		0.157 (0.096)	0.674 (0.598)		Bimodal pattern with morning and evening peaks
49	59.046	C₃H₆O	Acetone + Propanal		3.647 (2.162)	10.593 (8.481)		Bimodal pattern with afternoon and evening peaks
50	61.025	C₂H₄O₂	Acetic acid+ Glycolaldehyde		4.103 (3.342)	10.975 (8.781)		Trimodal pattern
51	69.031	C₄H₄O	Furan		0.032 (0.019)	0.168 (0.135)		Bimodal pattern with morning and evening peaks
52	71.047	C₄H₆O	Methyl Vinyl Ketone, Methacrolein, 2-Butenal		0.291 (0.189)	0.498 (0.419)		Bimodal pattern with morning and evening peaks
53	73.026	C₃H₄O₂	Methyl glyoxal		0.161 (0.109)	0.261 (0.259)		Unimodal pattern with afternoon peak
54	73.062	C₄H₈O	Butanal, 2-Butanone, MEK		0.555 (0.388)	1.418 (1.195)		Bimodal pattern with morning and evening peaks
55	75.042	C₃H₆O₂	Hydroxyacetone		0.278 (0.143)	1.012 (0.848)		Bimodal pattern with morning and evening peaks
56	81.031	C₅H₄O	2,4-Cyclopentadiene-1-one		0.014 (0.007)	0.06 (0.055)		Bimodal pattern with morning and evening peaks
57	83.047	C₅H₆O	2-Methyl furan		0.05 (0.026)	0.205 (0.157)		Bimodal pattern with morning and evening peaks
58	85.027	C₄H₄O₂	2-Furanone / butenedial		0.05 (0.034)	0.275 (0.213)		Bimodal pattern with afternoon

								and evening peaks
59	85.063	C₅H₈O	Cyclopentanone		0.06 (0.03)	0.167 (0.132)	Bimodal pattern with afternoon and evening peaks	
60	87.043	C₄H₆O₂	2,3 butanedione/ biacetyl		0.175 (0.094)	0.566 (0.465)	Bimodal pattern with afternoon and evening peaks	
61	87.079	C₅H₁₀O	2-Pentanone, 2-methyl-3-butene-2-ol, Pentanal		0.052 (0.031)	0.141 (0.132)	Bimodal pattern with afternoon and evening peaks	
62	89.058	C₄H₈O₂	Butanoic acid, Ethyl acetate		0.281 (0.234)	0.533 (0.449)	Bimodal pattern with morning and afternoon peaks	
63	95.048	C₆H₆O	Phenol		0.097 (0.057)	0.418 (0.352)	Trimodal pattern in monsoon while bimodal pattern with morning and evening peaks in post-monsoon	
64	97.027	C₅H₄O₂	Furfural		0.048 (0.036)	0.355 (0.294)	Bimodal pattern with morning and evening peaks	
65	97.063	C₆H₈O	C2 substituted furan, 2-methyl-2-Cyclopenten-1-one		0.034 (0.016)	0.132 (0.098)	Bimodal pattern with morning and evening peaks	
66	99.043	C₅H₆O₂	Furfuryl alcohol, 3-Methyl-2-furanone 4-Methyl-5H-furan-2-one		0.081 (0.059)	0.267 (0.251)	Unimodal pattern with afternoon peak	
67	99.079	C₆H₁₀O	Cyclohexanone		0.167 (0.109)	0.424 (0.346)	Bimodal pattern with afternoon and evening peaks	
68	101.059	C₅H₈O₂	2,3-Pentanedione, methyl methacrylate &		0.129 (0.074)	0.304 (0.268)	Bimodal pattern with afternoon and evening peaks	

				other hydrocarbons				
69	107.049	C₇H₆O	Benzaldehyde		0.06 (0.046)	0.202 (0.19)	Bimodal pattern with afternoon and evening peaks	
70	109.064	C₇H₈O	Methylphenol isomers, Anisole		0.027 (0.016)	0.1 (0.078)	Bimodal pattern with morning and evening peaks	
71	111.042	C₆H₆O₂	5-Methylfurfural, Hydroxyphenol		0.015 (0.01)	0.097 (0.083)	Trimodal pattern in monsoon while Bimodal pattern with morning and evening peak in post-monsoon	
72	111.08	C₇H₁₀O	C3-substituted furans, C2-substituted cyclopentene, methyl cyclohexene		0.021 (0.011)	0.081 (0.068)	Bimodal pattern with morning and evening peaks	
73	113.059	C₆H₈O₂	Dimethylbutenedial / C4-substituted aldehyde		0.047 (0.027)	0.159 (0.143)	Bimodal pattern with morning and evening peaks	
74	115.039	C₅H₆O₃	5-Hydroxymethyl-2-furanone/ methylepoxybutanedial		0.014 (0.01)	0.046 (0.046)	Unimodal pattern with afternoon peak	
75	115.075	C₆H₁₀O₂	C6 diketone isomers/ C6 esters		0.051 (0.028)	0.124 (0.121)	Unimodal pattern with afternoon peak	
76	121.064	C₈H₈O	Tolualdehyde		0.065 (0.046)	0.209 (0.195)	Bimodal pattern with afternoon and evening peaks	
77	123.044	C₇H₆O₂	2-Hydroxybenzaldehyde		0.027 (0.017)	0.119 (0.104)	Unimodal pattern with afternoon peak	
78	123.08	C₈H₁₀O	C2-substituted phenol, methyl anisole		0.015 (0.008)	0.054 (0.046)	Bimodal pattern with morning and evening peaks	
79	125.06	C₇H₈O₂	Guaiacol		0.016 (0.009)	0.06 (0.049)	Bimodal pattern with afternoon and evening peaks	

80		127.039	C₆H₆O₃	Hydroxymethyl furfural		0.009 (0.006)	0.044 (0.039)	Unimodal pattern with afternoon peak
81		127.075	C₇H₁₀O₂	Trimethylbutenedial / Methyl sorbate		0.025 (0.013)	0.077 (0.07)	Unimodal pattern with afternoon peak
82		129.092	C₇H₁₂O₂	C7-diketone/heptane-2,6-dione		0.025 (0.016)	0.051 (0.049)	Unimodal pattern with afternoon peak
83		133.065	C₉H₈O	Methyl benzofuran		0.007 (0.003)	0.027 (0.023)	Bimodal pattern with morning and evening peaks
84		135.08	C₉H₁₀O	3-Methylacetophenone		0.016 (0.01)	0.058 (0.054)	Bimodal pattern with morning and evening peaks
85		143.108	C₈H₁₄O₂	2,3-Octanedione		0.02 (0.011)	0.04 (0.035)	Unimodal pattern with afternoon peak
86		145.051	C₆H₈O₄	Organic acids/levoglucosan fragment		0.006 (0.003)	0.022 (0.018)	Unimodal pattern with afternoon peak
87		145.123	C₈H₁₆O₂	n-Octanoic acid		0.009 (0.006)	0.019 (0.014)	Unimodal pattern with afternoon peak in monsoon while bimodal pattern with afternoon and evening peak in post-monsoon
88		149.024	C₈H₄O₃	Phthalic anhydride/ 2,3-Benzofurandione		0.014 (0.011)	0.062 (0.059)	Unimodal pattern with afternoon peak
89		149.096	C₁₀H₁₂O	Methyl chavicol (estragole)		0.007 (0.004)	0.03 (0.027)	Bimodal pattern with morning and evening peaks
90		153.092	C₉H₁₂O₂	Oxonopinone		0.009 (0.004)	0.029 (0.026)	Bimodal pattern with afternoon and evening peaks
91		153.128	C₁₀H₁₆O	Camphor pinene oxide		0.022 (0.015)	0.096 (0.086)	Bimodal pattern with afternoon and evening peaks
92		155.108	C₉H₁₄O₂	Norpinonaldehyde		0.012 (0.006)	0.026 (0.022)	Unimodal pattern with afternoon peak

93		155.144	C₁₀H₁₈O	Cineole, Linalool, 4- tert-butyl cyclohexanone		0.01 (0.007)	0.023 (0.019)	Unimodal pattern with afternoon peak in monsoon while bimodal pattern with afternoon and evening peak in post-monsoon
94		157.122	C₉H₁₆O₂	C9- ester		0.013 (0.007)	0.026 (0.023)	Unimodal pattern with afternoon peak
95		159.14	C₉H₁₈O₂	C9-organic acid		0.007 (0.005)	0.013 (0.01)	Unimodal pattern with afternoon peak
96		177.056	C₁₀H₈O₃	2- Formylcinnami c acid / hydroxy- methyl- coumarin		0.008 (0.005)	0.026 (0.022)	Bimodal pattern with afternoon and evening peaks
97		185.121	C₁₀H₁₆O₃	cis-Pinonic acid		0.006 (0.004)	0.01 (0.008)	Unimodal pattern with afternoon peak
98		195.138	C₁₂H₁₈O₂	Myrtenyl acetate		0.002 (0.001)	0.006 (0.006)	Unimodal pattern with afternoon peak
99		42.03	C₂H₃N	Acetonitrile		0.291 (0.126)	0.942 (0.714)	Bimodal pattern with morning and evening peaks
100		44.018	HNCO	Isocyanic acid	$\text{HN}=\text{C}=\text{O}$	0.051 (0.038)	0.139 (0.095)	Bimodal pattern with morning and afternoon peaks
101		46.025	CH₄NO	Formamide		0.232 (0.206)	0.296 (0.236)	Unimodal pattern with afternoon peak
102		48.048	CH₅NO	methoxyamine		0.003 (0.002)	0.01 (0.009)	Bimodal pattern with morning and evening peaks
103		76.037	C₂H₅NO₂	Nitroethane		0.009 (0.005)	0.213 (0.206)	Unimodal pattern with afternoon peak
104		84.08	C₅H₉N	Pentanenitrile/ Methylbutanen itrile isomers/ C5-amines		0.005 (0.003)	0.021 (0.022)	Bimodal pattern with morning and evening peaks

105		116.108	C₆H₁₃NO	C6-amide		0.006 (0.004)	0.01 (0.007)	Unimodal pattern with afternoon peak
106		124.039	C₆H₅NO₂	Nitrobenzene		0.006 (0.004)	0.019 (0.018)	Trimodal pattern
107		138.056	C₇H₇NO₂	Nitrotoluene/ salicylamide		0.003 (0.001)	0.013 (0.01)	Trimodal pattern
108		154.052	C₇H₇NO₃	Nitrobenzyl alcohol/Nitroresols, methyl-nitrophenol		0.005 (0.004)	0.024 (0.025)	Trimodal pattern
109	CIVOC S	62.997	C₂H₃Cl	Vinyl chloride		0.004 (0.003)	0.015 (0.011)	Bimodal pattern with afternoon and evening peaks
110		146.977	C₆H₄Cl₂	Dichlorobenzene		0.025 (0.021)	0.115 (0.121)	Bimodal pattern with morning and evening peaks
111	SVOC S	49.007	CH₄S	Methanethiol		0.048 (0.047)	0.128 (0.129)	Bimodal pattern with morning and evening peaks

- Bold ones in structure 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.

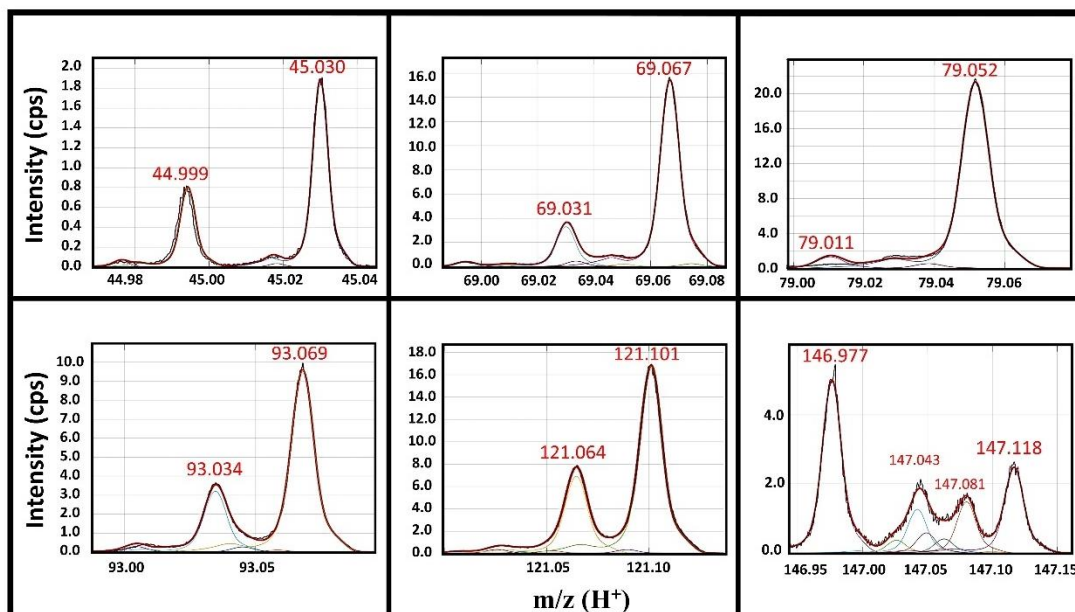
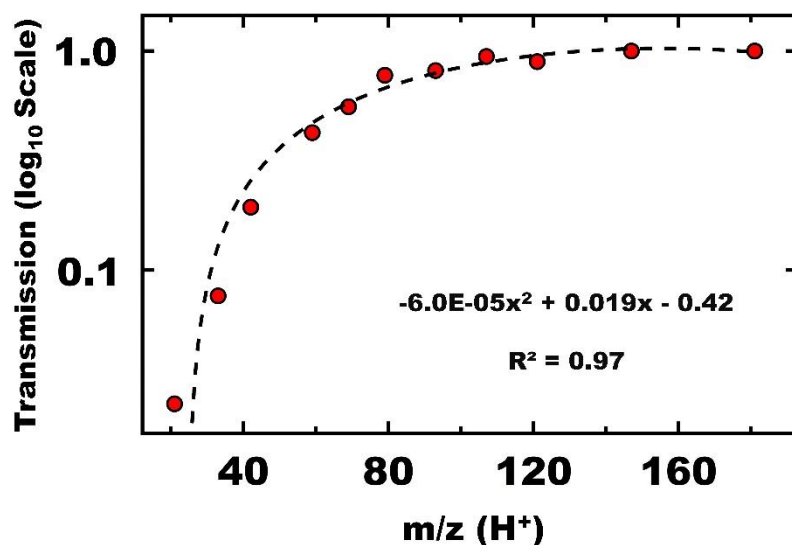


Figure S2: Transmission values as a function of m/z for the PTR-TOF-MS 10K obtained during a calibration experiment performed on 26th September 2022 using the VOC calibration gas mixture (Societa Italiana Acetilene E Derviat; S.I.A.D. S.p.A., Italy) containing 11 hydrocarbons at ~100 ppb, namely methanol, acetonitrile, acetone, isoprene, benzene, toluene, xylene, trimethylbenzene, and dichlorobenzene and trichlorobenzene



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

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_0 = Reduced mobility of H_3O^+ ions ($2.8 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$)

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

Figure S3 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.

