

Supplement information for-

Real-time measurements of NMVOCs in the central IGB, Lucknow, India: Source characterization and their role in O₃ and SOA formation

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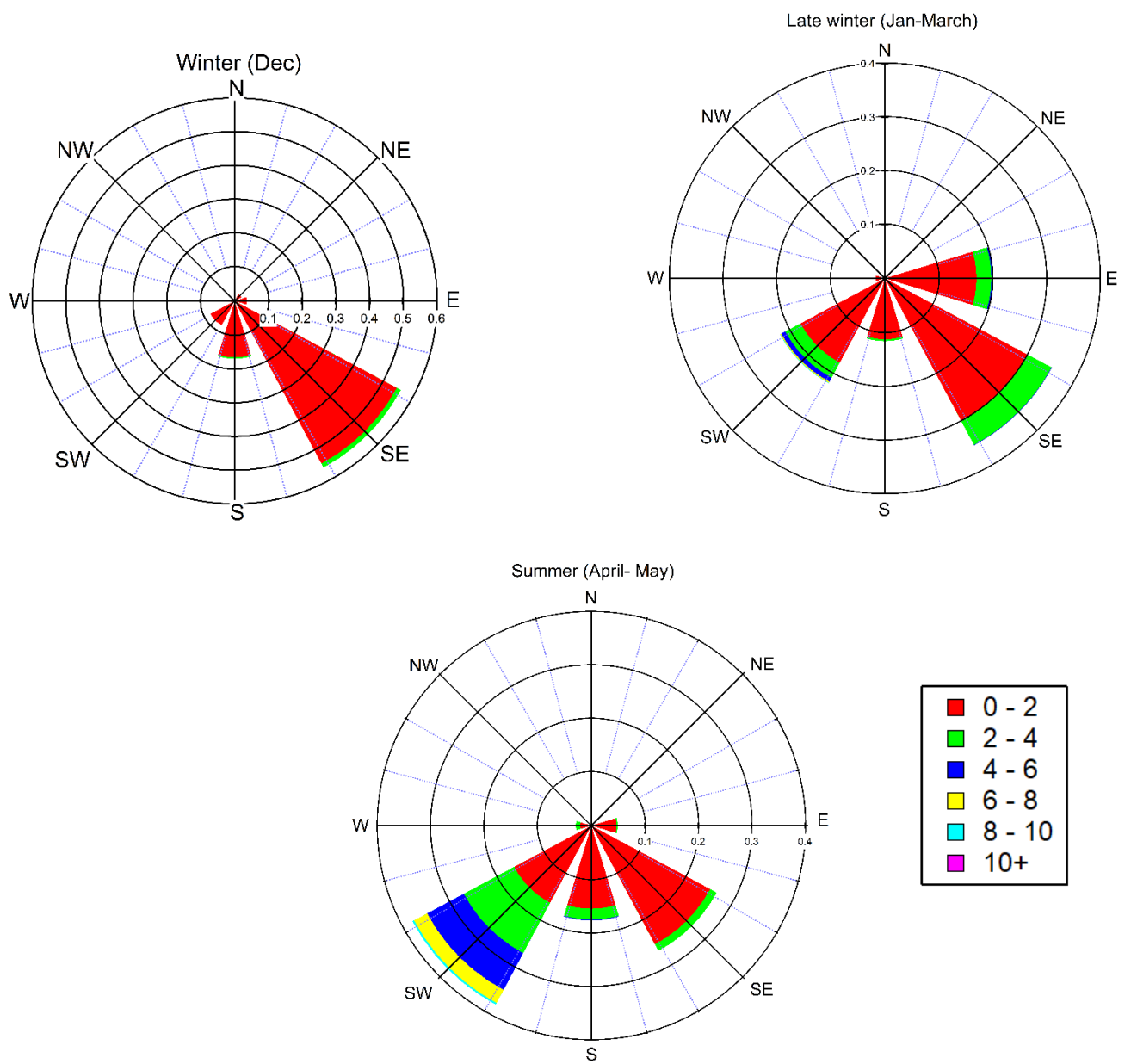


Figure S1: Wind rose plots showing wind speed and direction in different seasons at sampling site

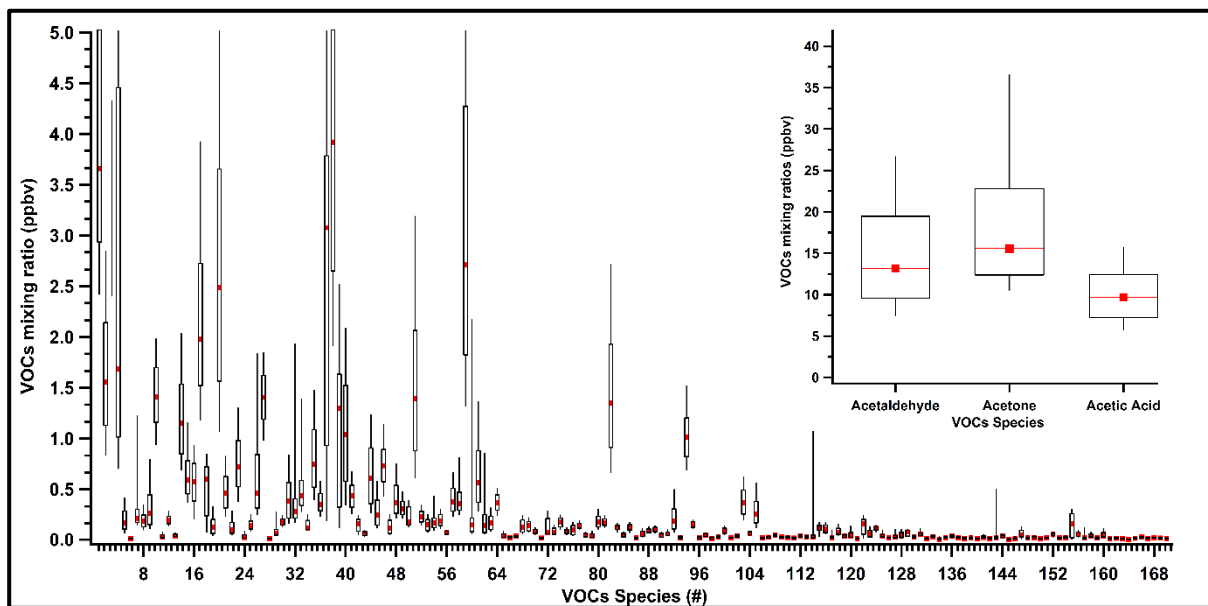
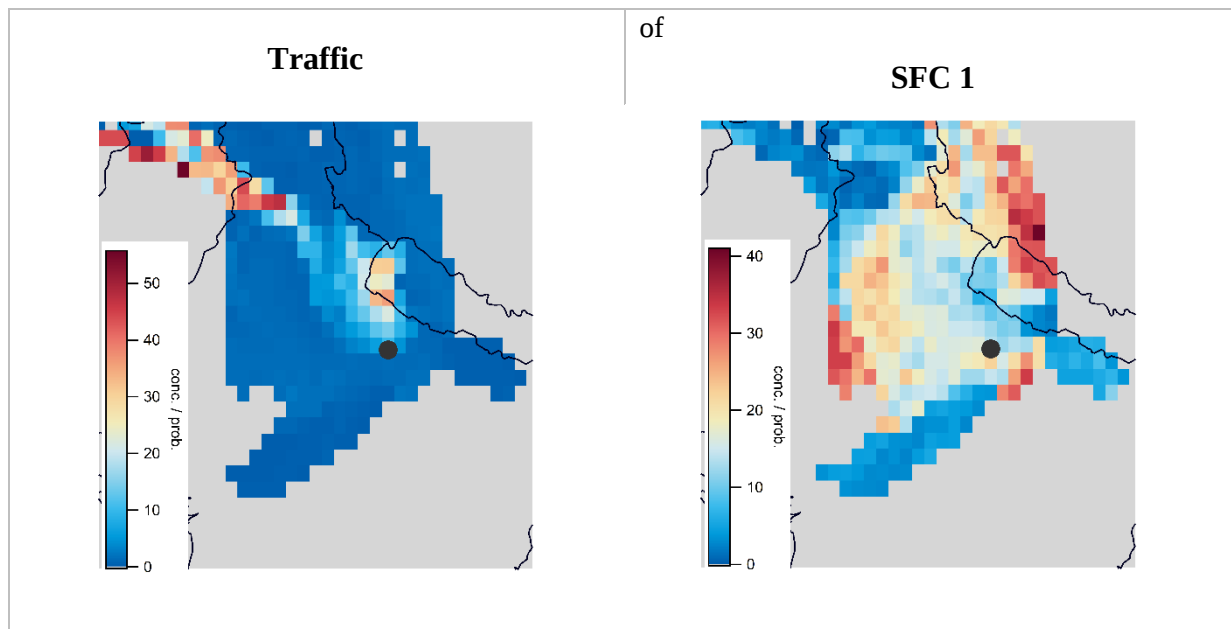


Figure S2: Box plots showing the concentrations individual NMVOCs over the whole study period. The Box represents the 25-75% inter-quartiles of the data with highest and lowest points as whiskers. The middle red box is the mean of the concentrations of individual NMVOCs.



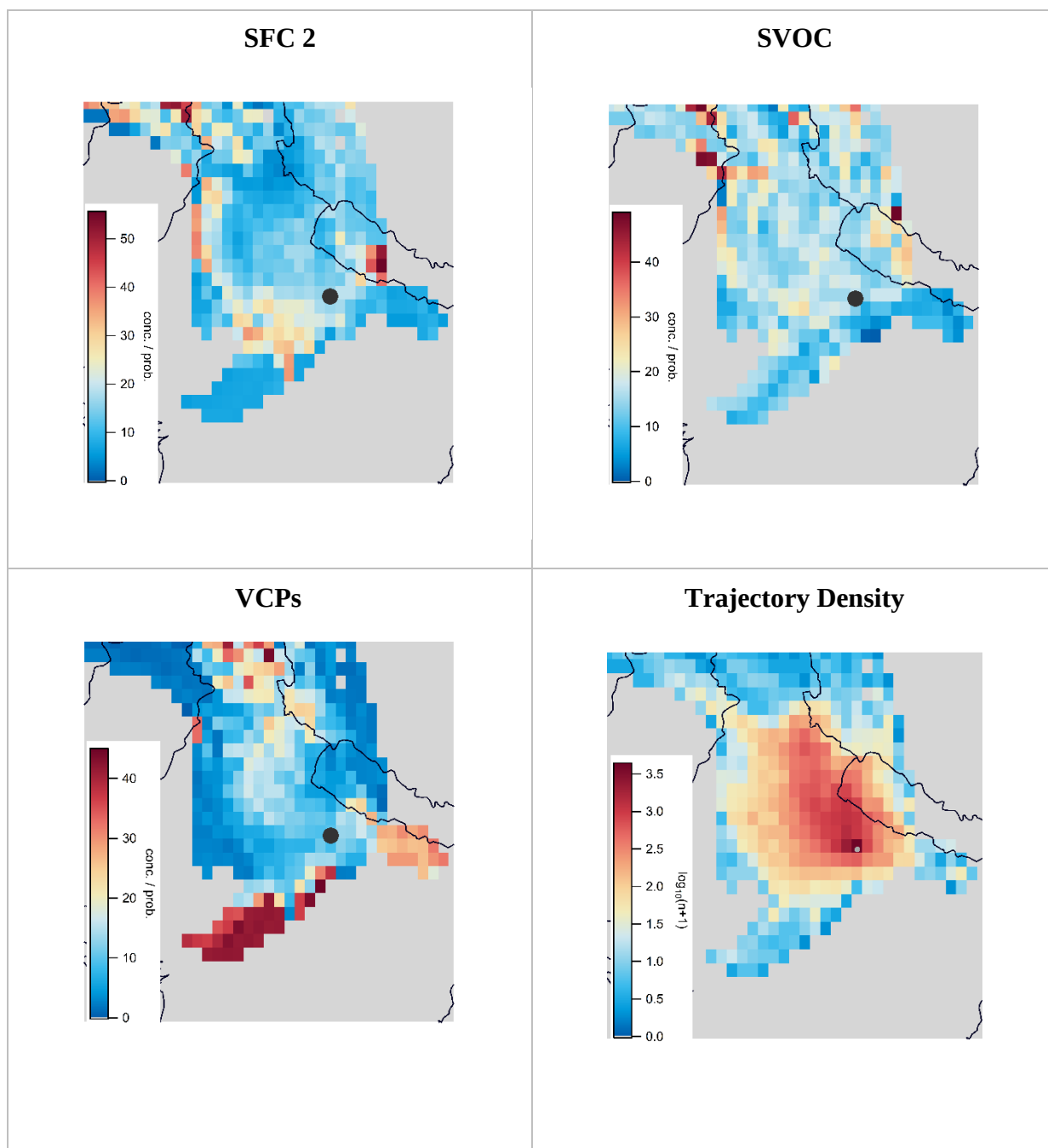


Figure S3: Graphs showing concentration weighted trajectories for individual factors (Traffic, SFC1, SFC 2, SVOC, VCPs), and trajectory density also for the sampling site in Lucknow.

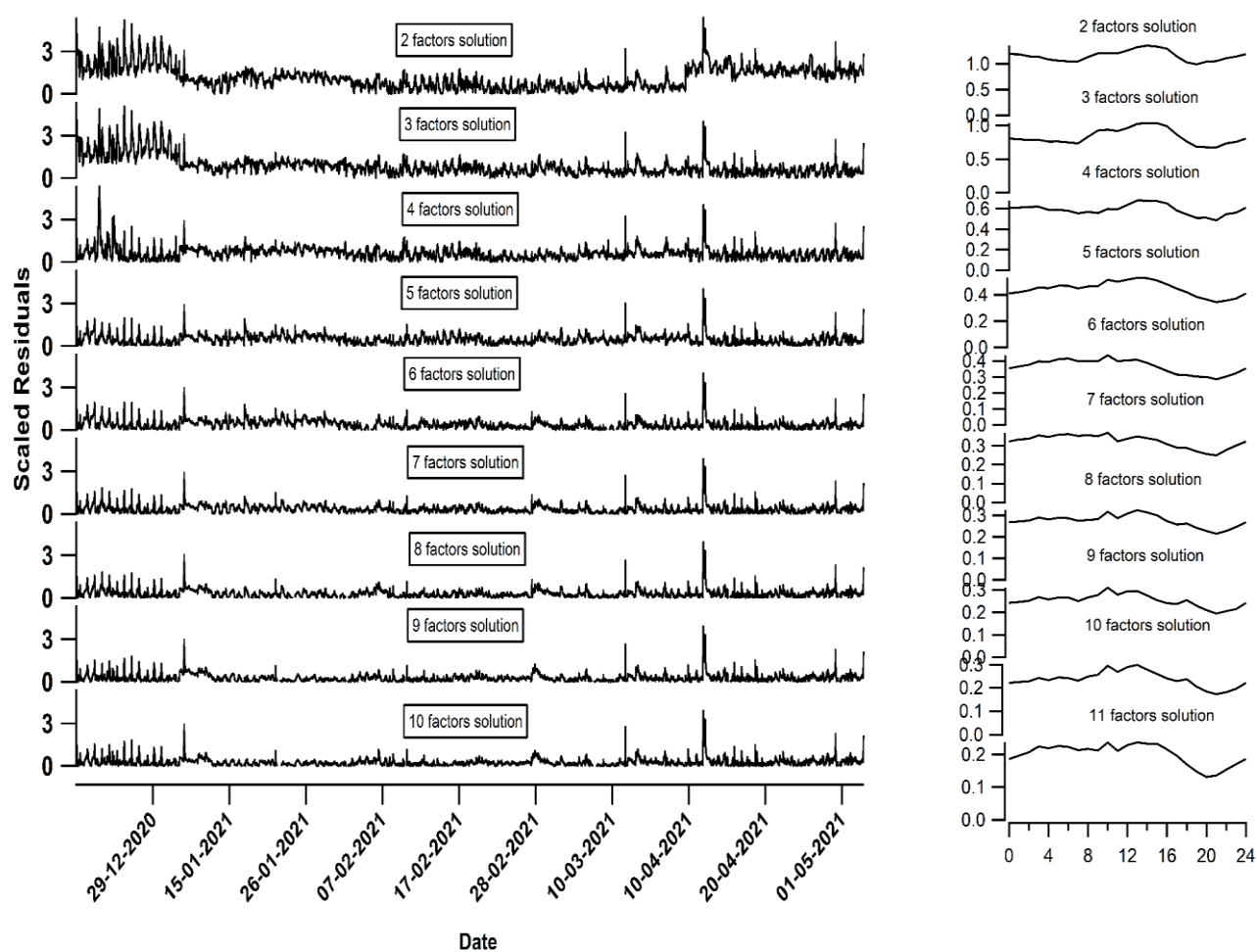


Figure S4: Timeseries and diurnal variation of the scaled residuals from 2-11 factors solution.

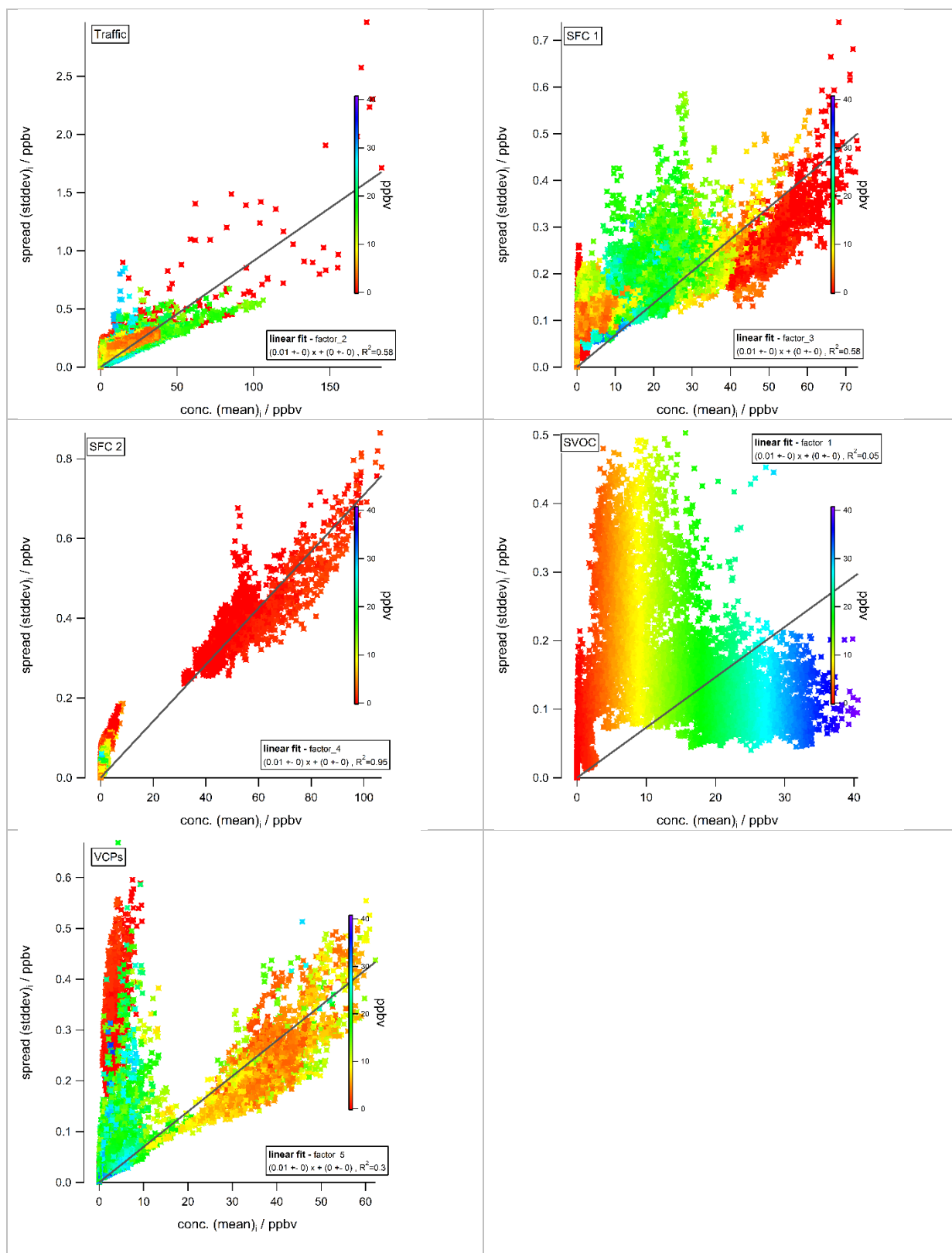


Figure S5: Mass estimation error for individual factors after bootstrap analysis.

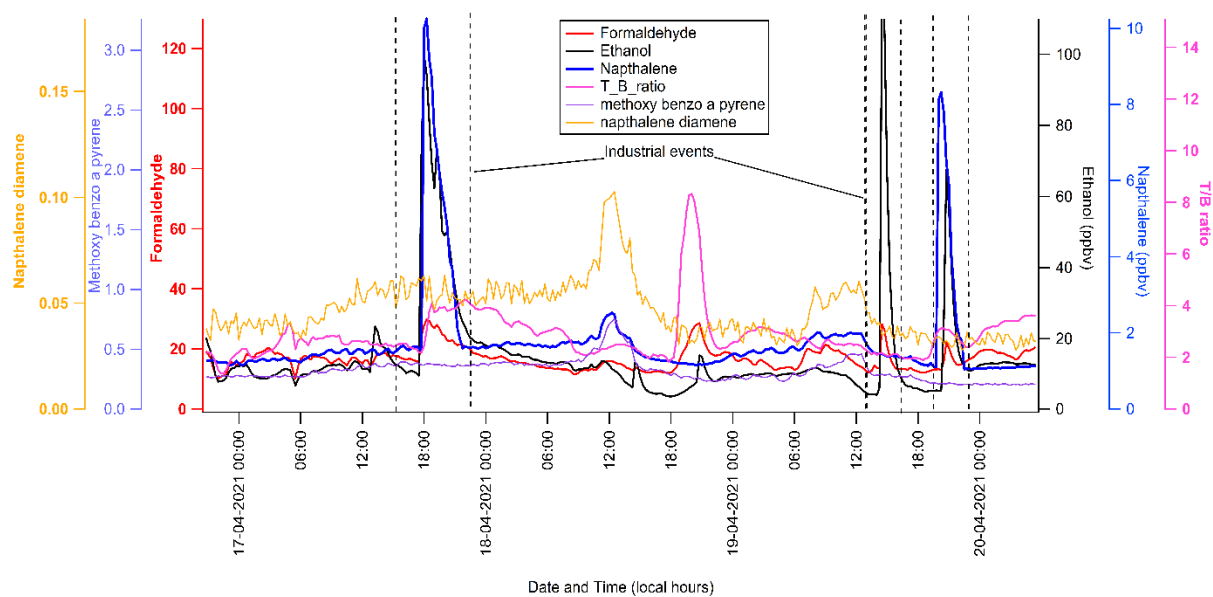


Figure S6: Timeseries of high-resolution data for showing particular peaks of industrial events

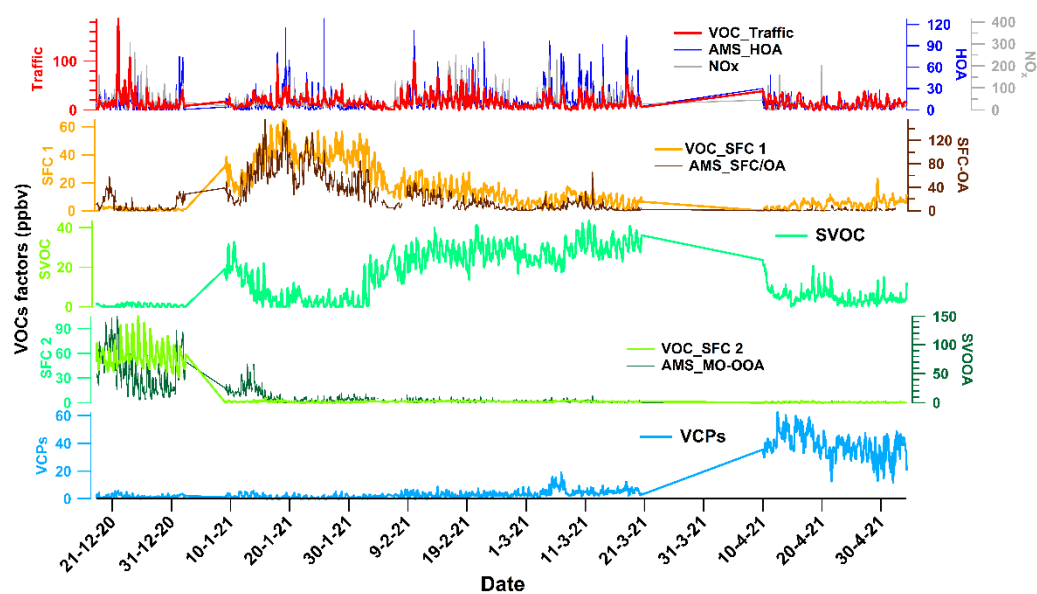


Figure S7: Timeseries of 5-factor solution of NMVOCs, correlated with AMS_organic aerosols resolved factors and NOx

Supplementary Table S1: List of 173 NMVOCs measured during the study period. The NMVOCs not included in PMF analysis are highlighted with grey shade. Column 2,3,4 contains the exact m/z value of the VOCs, the chemical formula for the particular m/z, and their probable species names. These names are adopted from previous studies and NIST book. Column 5 includes the family classification as discussed in the main text.

S. No.	m/z	Chemical formula	Species Name	Family
1	31.018	C1H3O1	Formaldehyde	CHO1
2	42.034	C2H4N1	Acetonitrile	CxHyNz
3	45.034	C2H5O1	Acetaldehyde	CHO1
4	47.012	C1H3O2	Formic acid	CHO2
5	47.049	C2H6O	Ethanol	CHO1
6	54.034	C3H4N1	Acrylonitrile	CxHyNz
7	59.049	C3H7O1	Acetone	CHO1
8	61.028	C2H5O2	Acetic acid	CHO2
9	67.021	C3H3N2	Malononitrile	CxHyNz
10	67.055	C5H7	1,3 cyclopentadiene`	N_CxHy
11	68.056	C4H6N1	Pyrole/Butenenitrile isomer	CxHyNz
12	69.033	C4H5O1	Furan	Furan
13	69.070	C5H9	Isoprene	N_CxHy
14	70.038	C2H4N3	Triazole	CxHyNz
15	70.073	C4H8N1	Butane nitrile	CxHyNz
16	71.014	C3H3O2	Propiolic acid	CHO2
17	71.049	C4H7O1	Methyl vinyl ketone	CHO1
18	71.085	C5H11	Pentene	N_CxHy
19	73.028	C3H5O2	Methylglyoxal, acrylic acid	CHO2
20	73.064	C4H9O1	Methyl ethyl ketone	CHO1
21	77.019	C2H5O3	Acetic acid	CHO3
22	77.048	C3H9O2	Propylene glycol	CHO2
23	79.053	C6H7	Benzene	Ar_CxHy
24	80.054	C5H6N1	Pyridine, C5 nitriles	CxHyNz
25	81.036	C5H5O1	Furfurals	Furan
26	81.070	C6H9	Cyclopentadiene	N_CxHy
27	82.041	C3H4N3	Triazine	CxHyNz
28	82.069	C5H8N1	C2 substituted pyrroles/Methylpyrole	CxHyNz
29	83.049	C5H7O1	Methylfuran	Furan
30	83.086	C6H11	Methylcyclohexene	N_CxHy
31	84.024	C2H2N3O1	Unknown	CxHyNzOn
32	84.055	C4H6N1O1	Butane nitrile	CxHyNzOn
33	84.086	C5H10N1	Pentane nitriles	CxHyNz
34	85.029	C4H5O2	Furanone	Furan
35	85.093	C6H13	Hexene/C6-alkene	N_CxHy
36	87.075	C5H11O1	Pentanone	CHO1
37	89.027	C3H5O3	Pyruvic acid	CHO3
38	89.058	C4H9O2	Ethyl acetate	CHO2
39	91.056	C7H7	Unknown	Others

40	93.033	C6H5O1	Unknown	CHO1
41	93.070	C7H9	Toluene	Ar_CxHy
42	95.015	C5H3O2	3-Cyclobutene-1,2-dione/Diketocyclobutene	CHO2
43	95.049	C6H7O1	Phenol	Phenol
44	95.086	C7H11	Unknown	Others
45	96.052	C5H6N1O1	Methylisoxazole	CxHyNzOn
46	96.091	C6H10N1	Dimethylpyrrole	CxHyNz
47	97.027	C5H5O2	Furaldehyde (furfural)	Furan
48	97.064	C6H9O1	C2- substituted furans/dimethyl furan	Furan
49	97.101	C7H13	Cycloheptene	N_CxHy
50	99.004	C4H3O3	Maleic anhydride/Furandione	Furan
51	99.043	C5H7O2	Furfuryl alcohol	Furan
52	99.080	C6H11O1	Cyclohexanone, hexanones	CHO1
53	101.022	C4H5O3	Dihydrofuranodione	Furan
54	101.059	C5H9O2	Methyl methacrylate	CHO2
55	101.095	C6H13O1	Hexanones/ Hexanal	CHO1
56	103.039	C4H7O3	Acetic anhydride	CHO3
57	103.075	C5H11O2	Unknown	CHO2
58	104.053	C7H6N1	Benzonitrile	CxHyNz
59	105.033	C7H5O1	Unknown	CHO1
60	105.071	C8H9	Styrene	Ar_CxHy
61	107.048	C7H7O1	Benzaldehyde	CHO1
62	107.086	C8H11	Xylene/ethylbenzene	Ar_CxHy
63	109.065	C7H9O1	Cresol (methylphenol)	Phenol
64	109.104	C8H13	Unknown	Others
65	111.043	C6H7O2	Catechol (Benzenediol)/ methyl furfural	Phenol
66	111.079	C7H11O1	C3 substituted furan	Furan
67	111.115	C8H15	Unknown	Others
68	112.046	C5H6N1O2	Methylmaleimide	CxHyNzOn
69	112.081	C5H10N3	Histamine	CxHyNz
70	112.118	C7H14N1	Heptanonitrile	CxHyNz
71	113.022	C5H5O3	5-Hydroxy 2-furfural	Furan
72	113.058	C6H9O2	2-hydroxy-3-methyl-2- cyclopentenone	Furan
73	113.096	C7H13O1	Cycloheptanone	CHO1
74	113.136	C8H17	Octene	N_CxHy
75	115.012	C3H3N2O3	Unknown	CxHyNzOn
76	115.038	C5H7O3	Hydroxymethyl furanone	Furan
77	115.075	C6H11O2	Unknown	CHO2
78	115.111	C7H15O1	Heptanal	CHO1
79	117.057	C5H9O3	Unknown	CHO3
80	117.090	C6H13O2	Unknown	CHO2
81	118.070	C8H8N1	Benzene acetonitrile	CxHyNz
82	119.043	C8H7O1	Benzofuran	Furan
83	119.086	C9H11	Methylstyrene/indane	N_CxHy
84	121.061	C8H9O1	Vinylphenol	Phenol

85	121.102	C9H13	Trimethylbenzene	Ar_CxHy
86	123.044	C7H7O2	Salicylaldehyde	Phenol
87	123.081	C8H11O1	Xylenol/ Ethylphenol/dimethylphenol	Phenol
88	123.117	C9H15	Allylcyclohexene	N_CxHy
89	125.024	C6H5O3	Hydroxybenzoquinone	CHO3
90	125.059	C7H9O2	Guaiacol	phenol
91	125.096	C8H13O1	Butyl furan	Furan
92	125.133	C9H17	Nonyne	N_CxHy
93	127.037	C6H7O3	Hydroxymethylfurfural	Furan
94	127.075	C7H11O2	Unknown	CHO2
95	127.111	C8H15O1	Octenal	CHO1
96	127.151	C9H19	Nonene	N_CxHy
97	129.056	C10H9	Napthalene	Ar_CxHy
98	129.118	C8H17O1	Octanal	CHO1
99	131.064	C6H11O3	Ethyl acetoacetate	CHO3
100	131.089	C10H11	Dihydronapthalene	Ar_CxHy
101	131.123	C6H15N2O1		CxHyNzOn
102	133.060	C9H9O1	Methylbenzofuran	Furan
103	133.101	C10H13	Dicyclopentadiene	N_CxHy
104	135.042	C8H7O2	Unknown	CHO2
105	135.075	C9H11O1	Unknown	CHO1
106	135.117	C10H15	Cymene	Ar_CxHy
107	137.061	C8H9O2	Unknown	CHO2
108	137.134	C10H17	Pinene	N_CxHy
109	139.032	C6H7N2O2	Unknown	CxHyNzOn
110	139.071	C8H11O2	Methylguaiacol	Phenol
111	139.110	C9H15O1	Pentylfuran	Furan
112	139.149	C10H19	Dicyne	N_CxHy
113	140.033	C6H6N1O3	Nitrophenol	CxHyNzOn
114	141.028	C4H5N4O2	Unknown	CxHyNzOn
115	141.091	C8H13O2	Unknown	CHO2
116	141.138	C9H17O1	Nonenal	CHO1
117	143.045	C6H7O4	Unknown	Others
118	143.103	C8H15O2	Unknown	CHO2
119	143.142	C9H19O1	Nonanal	CHO1
120	145.052	C6H9O4	Levogluconan pyrolysis product	Others
121	145.117	C8H17O2	Octanoic acid	CHO2
122	147.063	C6H11O4	Dehydropantoate	Others
123	147.114	C6H15N2O2	Nitro hexyl amine	CxHyNzOn
124	148.123	C10H14N1	Phenylpyrrolidine	CxHyNz
125	149.030	C7H5N2O2	Unknown	CxHyNzOn
126	149.084	C7H9N4	Unknown	CxHyNz
127	149.133	C11H17	C11 aromatics	Ar_CxHy
128	150.052	C11H4N1	Unknown	CxHyNz
129	150.130	C10H16N1	Phentermine	CxHyNz
130	151.047	C8H7O3	Piperonal	CHO3

131	151.151	C11H19	Unknown	Others
132	153.052	C8H9O3	Vanillin	CHO3
133	153.089	C9H13O2	Ethylguaiacol	Phenol
134	153.127	C10H17O1	Decadienal	CHO1
135	153.164	C11H21	Undycene	Others
136	154.054	C7H8N1O3	Methyl nitro phenol	CxHyNzOn
137	154.158	C9H16N1O1	Nonymamide	CxHyNzOn
138	155.069	C8H11O3	Syringol	phenol
139	155.105	C12H11	Heptalene	N_CxHy
140	155.149	C9H19N2	Unknown	CxHyNz
141	159.079	C11H11O1	Methoxynaphthalene	CHO1
142	159.102	C10H11N2	Naphthalenediamine	CxHyNz
143	161.092	C11H13O1	Unknown	CHO1
144	161.131	C12H17	Cyclohexylbenzene	Ar_CxHy
145	163.051	C9H7O3	Unknown	CHO3
146	163.115	C10H11O2	Phenyl butanedione	CHO2
147	163.165	C12H19	C12 aromatics	Ar_CxHy
148	165.054	C9H9O3	Unknown	CHO3
149	165.089	C10H13O2	Eugenol/isoegenol	Ar_CxHy
150	165.126	C12H21	Cyclododecyne	N_CxHy
151	167.034	C6H7N4O2	Unknown	CxHyNzOn
152	167.107	C10H15O2	Propylguaiacol	Phenol
153	167.175	C12H23	Dodecyne	N_CxHy
154	168.064	C8H10N1O3	Dimethyl nitrophenol	CxHyNzOn
155	169.096	C9H13O3	Trimethoxybenzene	CHO3
156	170.102	C12H12N1	Diphenylamine	CxHyNz
157	175.146	C13H19	Cycloheptane	Others
158	177.056	C10H9O3	Herniarin/methoxy benzopyranone	CHO3
159	177.162	C13H21	Heptylbenzene	Ar_CxHy
160	179.112	C11H15O2	Butyl benzoate	CHO2
161	179.179	C13H23	Triene	N_CxHy
162	181.124	C12H9N2	Phenazine	CxHyNz
163	183.102	C13H11O1	Benzylphenol	Phenol
164	185.134	C10H17O3	Unknown	CHO3
165	185.189	C12H25O1	Dodecanal	CHO1
166	189.042	C11H9O3	Unknown	CHO3
167	189.092	C12H13O2	Dimethoxynaphthalene	Ar_CxHy
168	189.157	C14H21	Unknown	Others
169	193.193	C14H25	Anthracene	N_CxHy
170	195.102	C11H15O3	Phenol, dimethoxy- propenyl	Phenol
171	195.174	C14H27	Tetradecyne	Others
172	197.138	C15H17	Unknown	Others
173	197.216	C14H29	Tetradecene	N_CxHy

Supplementary Table S2: List of NMVOCs with their MIR values (adopted from Carter, 2009) for estimating ozone formation potential (OFP)

Species name	Carbon number	Mir values carter, 2009	Species name	Carbon number	Mir values carter, 2009
Formaldehyde	1	9.59	Phenol	6	2.75
Acetonitrile	2	10.94	Furaldehyde (furfural)	5	7.01
Acrylonitrile	3	2.18	Hexanones/ hexanal	6	4.26
1,3 cyclopentadiene`	5	6.89	Styrene	8	1.66
Furan	4	9.03	Benzaldehyde	7	-0.71
Isoprene	5	10.48	Xylene/ethylbenzene	8	2.96
Methyl vinyl ketone	4	9.56	Cresol (methylphenol)	7	2.4
Methylglyoxal, acrylic acid	3	11.38	Cycloheptanone/c7 aldehyde	7	3.6
Methyl ethyl ketone	4	1.45	Octene	8	3.14
Acetic acid	2	0.67	Methylstyrene/indane	9	0.94
Propylene glycol	3	2.5	Vinylphenol	8	1.44
Benzene	6	0.69	Trimethylbenzene	9	1.96
Cyclopentadiene	6	6.89	Napthalene	10	3.28
Methylfuran	5	8.2	Octanal	8	3.08
Methylcyclohexene	6	4.89	Dicyclopentadiene	10	1.31
Hexene/c6-alkene	6	5.35	Cymene	10	4.41
Pentanone	5	2.72	Pinene	10	4.49
Ethyl acetate	4	0.59	C11 aromatics	11	2.04
Toluene	7	3.93	Cycloheptane	13	1.8
			Tetradecene	14	1.27

Supplementary Table S3: List of NMVOCs and their SOA yield for estimating their contribution to the SOA formation

mz_n (Ion)	Species Name	mz_text (Ion's chemical formula)	SOA Yield
69.033	Furan	C4H5O1	0.05
71.049	Methyl Vinyl Ketone	C4H7O1	0.03
79.053	Benzene	C6H7	0.33
81.07	Cyclopentadiene	C6H9	0.32
83.049	Methylfuran	C5H7O1	0.07
83.086	methylcyclohexene	C6H11	0.32
87.075	Pentanone	C5H11O1	0.32
91.056	Unknown	C7H7	0.32
93.033	Unknown	C6H5O1	0.32
93.07	Toluene	C7H9	0.24
95.049	Phenol	C6H7O1	0.44
95.086	Unknown	C7H11	0.32
96.091	Dimethylpyrrole	C6H10N1	0.32

97.064	C2- substituted furans/dimethyl furan	C6H9O1	0.32
97.101	cycloheptene	C7H13	0.32
99.08	cyclohexanone, hexanones	C6H11O1	0.32
101.095	hexanones/ Hexanal	C6H13O1	0.32
104.053	Benzonitrile	C7H6N1	0.32
105.033	Unknown	C7H5O1	0.32
105.071	Styrene	C8H9	0.32
107.048	Benzaldehyde	C7H7O1	0.32
107.086	Xylene/ethylbenzene	C8H11	0.2
109.065	Cresol (methylphenol)	C7H9O1	0.36
109.104	Unknown	C8H13	0.32
111.043	Catechol (Benzenediol)/ methyl furfural	0.32	
111.079	C3 substituted furan	C7H11O1	0.32
111.115	Unknown	C8H15	0.32
112.118	Heptanonitrile	C7H14N1	0.32
113.058	2-Hydroxy-3-Methyl-2-Cyclopentenone	0.32	
113.096	Cycloheptanone	C7H13O1	0.32
113.136	Octene	C8H17	0.32
115.075	Unknown	C6H11O2	0.32
115.111	Heptanal	C7H15O1	0.32
117.09	Unknown	C6H13O2	0.32
118.07	Benzene acetonitrile	C8H8N1	0.32
119.043	Benzofuran	C8H7O1	0.32
119.086	methylstyrene/indane	C9H11	0.32
121.061	Vinylphenol	C8H9O1	0.32
121.102	Trimethylbenzene	C9H13	0.32
123.044	Salicylaldehyde	C7H7O2	0.32
123.081	Xylenol/ Ethylphenol/dimethylphenol	0.44	
123.117	allylcyclohexene	C9H15	0.32
125.024	Hydroxybenzoquinone	C6H5O3	0.32
125.059	Guaiacol	C7H9O2	0.45
125.096	Butyl furan	C8H13O1	0.32
125.133	Nonyne	C9H17	0.32
127.037	Hydroxymethylfurfural	C6H7O3	0.32
127.075	Unknown	C7H11O2	0.32
127.111	Octenal	C8H15O1	0.32
127.151	Nonene	C9H19	0.32
129.056	Napthalene	C10H9	0.52
129.118	Octanal	C8H17O1	0.32
131.064	Ethyl acetoacetate	C6H11O3	0.32
131.089	Dihydronapthalene	C10H11	0.32
131.123	Unknown	C6H15N2O1	0.32
133.06	Methylbenzofuran	C9H9O1	0.32

133.101	dicyclopentadiene	C10H13	0.32
135.042	Unknown	C8H7O2	0.32
135.075	Unknown	C9H11O1	0.32
135.117	Cymene	C10H15	0.32
137.061	Unknown	C8H9O2	0.32
137.134	Pinene	C10H17	0.32
139.032	Unknown	C6H7N2O2	0.32
139.071	methylguaiacol	C8H11O2	0.32
139.11	Pentylfuran	C9H15O1	0.32
139.149	Dicyne	C10H19	0.32
140.033	Nitrophenol	C6H6N1O3	0.32
141.028	Unknown	C4H5N4O2	0.32
141.091	Unknown	C8H13O2	0.32
141.138	Nonenal	C9H17O1	0.32
143.045	Unknown	C6H7O4	0.32
143.103	Unknown	C8H15O2	0.32
143.142	Nonanal	C9H19O1	0.32
145.052	Levoglucosan pyrolysis product	C6H9O4	0.32
145.117	Octanoic acid	C8H17O2	0.32
147.063	Dehydropantoate	C6H11O4	0.32
147.114	nitro hexyl amine	C6H15N2O2	0.32
148.123	Phenylpyrrolidine	C10H14N1	0.32
149.03	Unknown	C7H5N2O2	0.32
149.084	Unknown	C7H9N4	0.32
149.133	C11 aromatics	C11H17	0.32
150.052	Unknown	C11H4N1	0.32
150.13	Phentermine	C10H16N1	0.32
151.047	Piperonal	C8H7O3	0.32
151.151	Unknown	C11H19	0.32
153.052	Vanillin	C8H9O3	0.32
153.089	Ethylguaiacol	C9H13O2	0.32
153.127	Decadienal	C10H17O1	0.32
153.164	Undycene	C11H21	0.32
154.054	methyl nitro phenol	C7H8N1O3	0.32
154.158	Nonynamide	C9H16N1O1	0.32
155.069	Syringol	C8H11O3	0.26
155.105	Heptalene	C12H11	0.07
155.149	Unknown	C9H19N2	0.32
159.079	Methoxynapthalene	C11H11O1	0.32
159.102	Naphthalenediamine	C10H11N2	0.32
161.092	Unknown	C11H13O1	0.32
161.131	Cyclohexylbenzene	C12H17	0.32
163.051	Unknown	C9H7O3	0.32
163.115	phenyl butanedione	C10H11O2	0.32
163.165	C12 aromatics	C12H19	0.32

165.054	Unknown	C9H9O3	0.32
165.089	Eugenol/Isoeugenol	C10H13O2	0.32
165.126	cyclododecyne	C12H21	0.32
167.034	Unknown	C6H7N4O2	0.32
167.107	Propylguaiacol	C10H15O2	0.32
167.175	dodecyne	C12H23	0.32
168.064	dimethyl nitrophenol	C8H10N1O3	0.32
169.096	trimethoxybenzene	C9H13O3	0.32
170.102	Diphenylamine	C12H12N1	0.32
175.146	Cycloheptane	C13H19	0.32
177.056	Herniarin/methoxy benzopyranone	C10H9O3	0.32
177.162	Heptylbenzene	C13H21	0.32
179.112	Butyl benzoate	C11H15O2	0.32
179.179	Triene	C13H23	0.32
181.124	Phenazine	C12H9N2	0.32
183.102	Benzylphenol	C13H11O1	0.32
185.134	Unknown	C10H17O3	0.32
185.189	Dodecanal	C12H25O1	0.32
189.042	Unknown	C11H9O3	0.32
189.092	Dimethoxynaphthalene	C12H13O2	0.32
189.157	Unknown	C14H21	0.32
193.193	Anthracene	C14H25	0.32
195.102	Phenol, dimethoxy- propenyl	C11H15O3	0.32
195.174	Tetradecyne	C14H27	0.32
197.138	Unknown	C15H17	0.32
197.216	Tetradecene	C14H29	0.32