Supplementary material

Occurrence of Volatile and Semi-Volatile Organic Pollutants in the Russian Arctic Atmosphere: the International Siberian Shelf Study Expedition (ISSS-2020)

Dmitry S. Kosyakov [1,*], Irina S. Shavrina [2], Nikolay V. Ul'yanovskii [1], Dmitry E. Lakhmanov [1] and Albert T. Lebedev [1,2,*]

[1]Laboratory of Environmental Analytical Chemistry, Core Facility Center "Arktika", Northern (Arctic) Federal University, Arkhangelsk, Russia; d.kosyakov@marfu.ru (D.S.K.), i.shavrina@narfu.ru (I.S.S.), d.lahmanov@narfu.ru (D.E.L.), n.ulyanovsky@narfu.ru (N.V.U.)
[2]Department of Organic Chemistry, Lomonosov Moscow State University, Moscow, Russia; mocehops@ya.ru (A.T.L.)
* Correspondence: d.kosyakov@marfu.ru (D.S.K.); mocehops@ya.ru (A.T.L.).

Table S1. Coordinates of sampling points, atmospheric conditions and dates of air collection

Sample	N	E	T, °C	P, mbar	Date
1	65.12997	39.77980	0	1010	2020-11-01
2	66.74825	41.24093	1	1022	2020-10-29
3	68.31443	42.26230	7	1030	2020-09-28
4	69.03775	44.55755	8	1028	2020-09-28
5	70.72725	58.91977	6	1017	2020-09-29
6	73.07417	68.49302	-4	1023	2020-10-27
7	73.17033	72.95966	2	1008	2020-10-01
8	73.89687	79.29628	0	1015	2020-10-03
9	74.52932	81.70145	-3	1015	2020-10-25
10	77.10350	124.81520	-1	992	2020-10-07
11	76.54045	128.65190	-1	1000	2020-10-20
12	73.10122	130.30660	1	994	2020-10-18
13	72.98955	140.16710	1	990	2020-10-16
14	77.52217	143.42510	-1	1005	2020-10-11
15	74.90207	160.91870	-1	1016	2020-10-13
16	74.99010	160.98610	-2	1018	2020-10-13

Table S2. Target VOCs, corresponding quantifier ions and limits of detection and quantification

№	t_r, min	Compounds	CAS #	Formula	*m/z*	LOD ng/tube	LOD ng/m³ *	LOQ ng/m³ *
Halogenated alkanes and alkenes								
1	1.53	Allyl chloride	107–05–1	C_3H_5Cl	76.0074	0.16	80	260
2	1.64	Methylene chloride	75–09–2	CH_2Cl_2	48.9840	0.045	22.5	75
3	1.75	1,1-Dichloroethene	75–35–4	$C_2H_2Cl_2$	95.9528	0.04	20	66
4	1.81	1,1-Dichloroethane	75–34–3	$C_2H_4Cl_2$	62.9996	0.01	5	17
5	1.85	Chloroprene	126–99–8	C_4H_5Cl	88.0074	0.004	2	7
6	1.93	*cis*-1,2-Dichloroethene	156–59–2	$C_2H_2Cl_2$	95.9528	0.02	10	33
7	1.93	*trans*-1,2-Dichloroethene	156–60–5	$C_2H_2Cl_2$	95.9528	0.02	10	33
8	1.98	2,2-Dichloropropane	594–20–7	$C_3H_6Cl_2$	77.0153	0.005	2.5	8
9	2.02	Chloroform	67–66–3	$CHCl_3$	82.9449	0.006	3	10
10	2.19	1,1,1-Trichloroethane	71–55–6	$C_2H_3Cl_3$	96.9606	0.004	2	7
11	2.25	1,2-Dichloroethane	107–06–2	$C_2H_4Cl_2$	61.9918	0.008	4	13
12	2.26	1,1-Dichloropropene	563–58–6	$C_3H_4Cl_2$	74.9996	0.004	2	7
13	2.33	Carbon tetrachloride	56–23–5	CCl_4	116.9060	0.003	1.5	5
14	2.73	Trichloroethene	79–01–6	C_2HCl_3	131.9109	0.003	1.5	5
15	2.75	1,2-Dichloropropane	78–87–5	$C_3H_6Cl_2$	76.0074	0.01	5	17
16	3.36	*cis*-1,3-Dichloropropene	10061–01–5	$C_3H_4Cl_2$	74.9996	0.001	0.5	2
17	3.95	*trans*-1,3-Dichloropropene	10061–02–6	$C_3H_4Cl_2$	74.9996	0.01	5	17
18	4.19	1,1,2-Trichloroethane	79–00–5	$C_2H_3Cl_3$	96.9606	0.01	5	17
19	4.40	1,3-Dichloropropane	142–28–9	$C_3H_6Cl_2$	76.0074	0.01	5	17
20	4.99	Tetrachloroethene	127–18–4	C_2Cl_4	165.8717	0.003	1.5	5
21	6.61	1,1,1,2-Tetrachloroethane	630–20–6	$C_2H_2Cl_4$	130.9216	0.002	1	4
22	8.42	*cis*-1,4-Dichloro-2-butene	1476–11–5	$C_4H_6Cl_2$	88.0074	0.005	2.5	8
23	8.93	1,1,2,2-Tetrachloroethane	79–34–5	$C_2H_2Cl_4$	82.9450	0.002	1	4
24	9.11	1,2,3-Trichloropropane	96–18–4	$C_3H_5Cl_3$	74.99958	0.001	0.5	2
25	9.17	*trans*-1,4-Dichloro-2-butene	110–57–6	$C_4H_6Cl_2$	88.0074	0.01	5	17
26	10.80	Pentachloroethane	76–01–7	C_2HCl_5	166.8796	0.004	2	7
27	17.19	Hexachloro-1,3-butadiene	87–68–3	C_4Cl_6	224.8404	0.001	0.5	2
28	1.61	Iodomethane	74–88–4	CH_3I	141.9274	0.3	150	490
29	1.62	1,1,2-Trichlorotrifluoroethane	76–13–1	$C_2Cl_3F_3$	150.9323	0.045	22.5	75
30	2.02	Bromochloromethane	74–97–5	CH_2BrCl	129.9002	0.016	8	27
31	2.78	Dibromomethane	74–95–3	CH_2Br_2	173.8496	0.005	2.5	8
32	2.89	Bromodichloromethane	75–27–4	$CHBrCl_2$	82.9449	0.005	2.5	8
33	4.84	Dibromochloromethane	124–48–1	$CHBr_2Cl$	128.8921	0.006	3	10
34	5.13	1,2-Dibromoethane (EDB)	106–93–4	$C_2H_4Br_2$	106.9491	0.003	1.5	5
35	7.88	Bromoform	75–25–2	$CHBr_3$	172.8418	0.001	0.5	2
N-compounds								
36	1.61	Acrylonitrile	107–13–1	C_3H_3N	53.0260	0.25	125	410
37	1.78	Propionitrile	107–12–0	C_3H_5N	54.0339	0.04	20	66
38	1.93	Methacrylonitrile	126–98–7	C_4H_5N	67.0416	0.03	15	50
39	13.92	Nitrobenzene	98–95–3	$C_6H_5NO_2$	77.0386	0.003	1.5	5
S- and O-compounds								
40	1.66	Carbon disulfide	75–15–0	CS_2	75.9436	0.064	32	110
41	1.95	Methyl acrylate	96–33–3	$C_4H_6O_2$	85.0284	0.03	15	50

42	2.04	Isobutyl alcohol	78–83–1	$C_4H_{10}O$	43.0541	0.1	50	170
43	2.05	Tetrahydrofuran	109–99–9	C_4H_8O	71.0492	0.02	10	33
44	2.82	1,4-Dioxane	123–91–1	$C_4H_8O_2$	88.0518	0.003	1.5	5
45	2.86	Methyl methacrylate	80–62–6	$C_5H_8O_2$	99.0440	0.004	2	7
46	4.41	Ethyl methacrylate	97–63–2	$C_6H_{10}O_2$	99.0441	0.01	5	17
Aromatic hydrocarbons								
47	2.31	Benzene	71–43–2	C_6H_6	78.0464	0.003	1.5	5
48	3.90	Toluene	108–88–3	C_7H_8	91.0542	0.002	1	4
49	6.89	Ethylbenzene	100–41–4	C_8H_{10}	91.05425	0.001	0.5	2
50	7.20	*m*-Xylene	108–38–3	C_8H_{10}	91.05425	0.005	2.5	8
51	7.20	*p*-Xylene	95–47–6	C_8H_{10}	91.05425	0.005	2.5	8
52	7.93	Styrene	100–42–5	C_8H_8	104.0620	0.002	1	4
53	7.96	*o*-Xylene	106–42–3	C_8H_{10}	91.05425	0.003	1.5	5
54	9.01	Isopropylbenzene	98–82–8	C_9H_{12}	105.0699	0.001	0.5	2
55	10.00	*n*-Propylbenzene	103–65–1	C_9H_{12}	91.05424	0.001	0.5	2
56	10.51	1,3,5-Trimethylbenzene	108–67–8	C_9H_{12}	105.0698	0.002	1	4
57	11.18	*tert*-Butylbenzene	98–06–6	$C_{10}H_{14}$	119.0855	0.001	0.5	2
58	11.29	1,2,4-Trimethylbenzene	95–63–6	C_9H_{12}	105.0698	0.004	2	7
59	11.73	*sec*-Butylbenzene	135–98–8	$C_{10}H_{14}$	105.0699	0.002	1	4
60	12.21	4-Isopropyltoluene	99–87–6	$C_{10}H_{14}$	119.0855	0.002	1	4
61	13.11	n-Butylbenzene	104–51–8	$C_{10}H_{14}$	91.0542	0.003	1.5	5
Halogenated aromatic hydrocarbons								
62	6.35	Chlorobenzene	108–90–7	C_6H_5Cl	112.0074	0.002	1	4
63	9.20	Bromobenzene	108–86–1	C_6H_5Br	155.9568	0.004	2	7
64	9.86	2-Chlorotoluene	95–49–8	C_7H_7Cl	126.0231	0.004	2	7
65	10.12	4-Chlorotoluene	106–43–4	C_7H_7Cl	126.0231	0.005	2.5	8
66	11.58	1,3-Dichlorobenzene	541–73–1	$C_6H_4Cl_2$	145.9684	0.005	2.5	8
67	11.87	1,4-Dichlorobenzene	106–46–7	$C_6H_4Cl_2$	145.9684	0.005	2.5	8
68	12.38	1,2-Dichlorobenzene	95–50–1	$C_6H_4Cl_2$	145.9684	0.003	1.5	5
69	13.98	1,2-Dibromo-3-chloropropane	96–12–8	$C_3H_5Br_2Cl$	74.9996	0.003	1.5	5
70	16.31	1,2,4-Trichlorobenzene	120–82–1	$C_6H_3Cl_3$	179.9293	0.001	0.5	2
71	17.11	1,2,3-Trichlorobenzene	87–61–6	$C_6H_3Cl_3$	179.9294	0.001	0.5	2

* - recalculated for air sample volume of 2L

Table S3. Target SVOCs, corresponding quantifier ions and limits of detection and quantification

№	t_r, min	Compounds	CAS #	Formula	*m/z*	*LOD*	*LOD*	*LOQ*
						ng/tube	ng/m³	
N-compounds								
72	3.35	N-Nitrosodimethylamine	62–75–9	$C_2H_6N_2O$	74.0474	0.02	10	33
73	3.39	Pyridine	110–86–1	C_5H_5N	79.0416	0.01	5	17
74	10.72	Aniline	62–53–3	$C_6H_5NH_2$	93.0573	0.01	5	17
75	13.50	N-Nitroso-di-n-propylamine	621–64–7	$C_6H_{14}N_2O$	113.1073	0.006	3	10
76	15.12	2-Nitrophenol	88–75–5	$C_6H_5NO_3$	139.0263	0.01	5	17
77	16.95	4-Chloroaniline	106–47–8	$C_6H_4NH_2Cl$	127.0183	0.02	10	33
78	21.58	2-Nitroaniline	88–74–4	$C_6H_6N_2O_2$	138.0423	0.021	10.5	35
79	22.17	1,4-Dinitrobenzene	100–25–4	$C_6H_4N_2O_4$	168.0164	0.045	22.5	74
80	22.42	1,3-Dinitrobenzene	99–65–0	$C_6H_4N_2O_4$	168.0164	0.03	15	50
81	22.62	2,6-Dinitrotoluene	606–20–2	$C_7H_6N_2O_4$	165.0294	0.005	2.5	8
82	22.74	1,2-Dinitrobenzene	528–29–0	$C_6H_4N_2O_4$	168.0164	0.06	30	99
83	23.20	3-Nitroaniline	99–09–2	$C_6H_6N_2O_2$	138.0423	0.1	50	170
84	23.62	2,4-Dinitrophenol	51–28–5	$C_6H_4N_2O_5$	184.0113	0.85	425	1400
85	24.13	2,4-Dinitrotoluene	121–14–2	$C_7H_6N_2O_4$	165.0294	0.008	4	13
86	25.55	4-Nitroaniline	100–01–6	$C_6H_6N_2O_2$	138.0423	0.5	250	830
87	25.67	4,6-Dinitro-2-methylphenol	534–52–1	$C_7H_6N_2O_5$	198.0269	0.5	250	830
88	25.97	Diphenylamine	122–39–4	$C_{12}H_{11}N$	169.0886	0.006	3	10
89	26.07	Azobenzene	103–33–3	$C_{12}H_{10}N_2$	182.0838	0.003	1.5	5
90	29.88	Carbazole	86–74–8	$C_{12}H_9N$	167.0727	0.01	5	17
CHO-compounds								
91	10.90	Phenol	108–95–2	C_6H_6O	94.0413	0.004	2	7
92	12.55	Benzyl alcohol	100–51–6	C_7H_8O	79.0542	0.01	5	17
93	13.05	2-Methylphenol	95–48–7	C_7H_8O	108.0569	0.004	2	7
94	13.67	3-Methylphenol	108–39–4	C_7H_8O	108.0569	0.01	5	17
95	13.67	4-Methylphenol	106–44–5	C_7H_8O	108.0569	0.01	5	17
96	15.60	2,4-Dimethylphenol	105–67–9	$C_8H_{10}O$	122.0726	0.02	10	33
97	16.29	Benzoic acid	65-85-0	$C_7H_6O_2$	122.0363	0.3	148	490
Halogenated SVOCs								
98	11.08	2-Chlorophenol	95–57–8	C_6H_5OCl	128.0023	0.005	2.5	8
99	16.07	2,4-Dichlorophenol	120–83–2	$C_6H_4Cl_2O$	161.9632	0.02	10	33
100	19.03	4-Chloro-3-methylphenol	59–50–7	C_7H_7ClO	142.0179	0.015	7.5	25
101	20.52	2,4,6-Trichlorophenol	95–95–4	$C_6H_3Cl_3O$	195.9243	0.006	3	10
102	20.62	2,4,5-Trichlorophenol	88–06–2	$C_6H_3Cl_3O$	195.9243	0.008	4	13
103	24.39	2,3,5,6-Tetrachlorophenol	935–95–5	$C_6H_2Cl_4O$	231.8822	0.02	10	33
104	24.55	2,3,4,6-Tetrachlorophenol	58–90–2	$C_6H_2Cl_4O$	231.8822	0.015	7.5	25
105	25.49	4-Chlorophenyl phenyl ether	7005–72–3	$C_{12}H_9ClO$	204.0335	0.002	1	4
106	28.23	Pentachlorophenol	87–86–5	C_6HCl_5O	265.8432	0.13	65	210
107	11.07	Bis(2-chloroethyl)ether	111–44–4	$C_4H_8Cl_2O$	62.9996	0.006	3	10
108	13.57	Hexachloroethane	67–72–1	C_2Cl_6	200.8407	0.001	0.5	2
109	15.92	Bis(2-chloroethoxy)methane	111–91–1	$C_5H_{10}Cl_2O_2$	93.0102	0.004	2	7
110	19.91	Hexachlorocyclopentadiene	77–47–4	C_5Cl_6	236.8405	0.042	21	70
111	21.02	2-Chloronaphthalene	91–58–7	$C_{10}H_7Cl$	162.0229	0.001	0.5	2
112	27.37	Hexachlorobenzene	118–74–1	C_6Cl_6	283.8093	0.003	1.5	5

Polycyclic aromatic hydrocarbons								
113	16.51	Naphthalene	91–20–3	$C_{10}H_8$	128.0620	0.001	0.5	2
114	19.21	2-Methylnaphthalene	91–57–6	$C_{11}H_{10}$	141.0699	0.001	0.5	2
115	19.56	1-Methylnaphthalene	90–12–0	$C_{11}H_{10}$	141.0699	0.001	0.5	2
116	22.55	Acenaphthylene	208–96–8	$C_{12}H_8$	152.0619	0.001	0.5	2
117	23.26	Acenaphthene	83–32–9	$C_{12}H_{10}$	153.0698	0.001	0.5	2
118	23.94	Dibenzofuran	53–70–3	$C_{12}H_8O$	168.0568	0.001	0.5	2
119	25.25	Fluorene	86–73–7	$C_{13}H_{10}$	165.0697	0.001	0.5	2
120	28.89	Phenanthrene	85–01–8	$C_{14}H_{10}$	178.0773	0.013	6.5	22
121	29.09	Anthracene	120–12–7	$C_{14}H_{10}$	178.0773	0.004	2	7
122	33.47	Fluoranthene	206–44–0	$C_{16}H_{10}$	202.0772	0.002	1	4
123	34.27	Pyrene	129–00–0	$C_{16}H_{10}$	202.0772	0.002	1	4
124	38.97	Benz[a]anthracene	56–55–3	$C_{18}H_{12}$	228.0931	0.02	10	33
125	39.09	Chrysene	218–01–9	$C_{18}H_{12}$	228.0931	0.015	7.5	25
126	42.94	Benzo[b]fluoranthene	205–99–2	$C_{20}H_{12}$	252.0929	0.05	25	83
127	43.03	Benzo[k]fluoranthene	207–08–9	$C_{20}H_{12}$	252.0929	0.04	20	66
128	43.93	Benzo[a]pyrene	50–32–8	$C_{20}H_{12}$	252.0929	0.16	80	260
129	48.27	Benzo[g,h,i]perylene	191–24–2	$C_{22}H_{12}$	276.0929	0.85	425	1400
Phthalates								
130	22.51	Dimethylphthalate	131–11–3	$C_{10}H_{10}O_4$	163.0388	0.002	1	4
131	25.32	Diethylphthalate	84–66–2	$C_{12}H_{14}O_4$	149.0232	0.001	0.5	2
132	31.78	Di-*n*-butyl phthalate	84–74–2	$C_{16}H_{22}O_4$	149.0232	0.001	0.5	2
133	37.49	Benzyl butyl phthalate	85–68–7	$C_{19}H_{20}O_4$	149.0232	0.002	1	4
134	38.17	Bis(2-ethylhexyl)adipate	103–23–1	$C_{22}H_{42}O_4$	129.0545	0.015	7.5	25
135	40.01	Bis(2-ethylhexyl)phthalate	117–81–7	$C_{24}H_{38}O_4$	149.0232	0.002	1	3.3
136	42.42	Di-*n*-octyl phthalate	117–84–0	$C_{24}H_{38}O_4$	149.0232	0.01	5	17
Br-compounds								
137	27.33	4-Bromophenyl phenyl ether	101–55–3	$C_{12}H_9BrO$	247.9828	0.003	1.5	5
O-compounds								
138	14.87	Isophorone	78–59–1	$C_9H_{14}O$	82.0412	0.001	0.5	2

* - recalculated for air sample volume of 2L

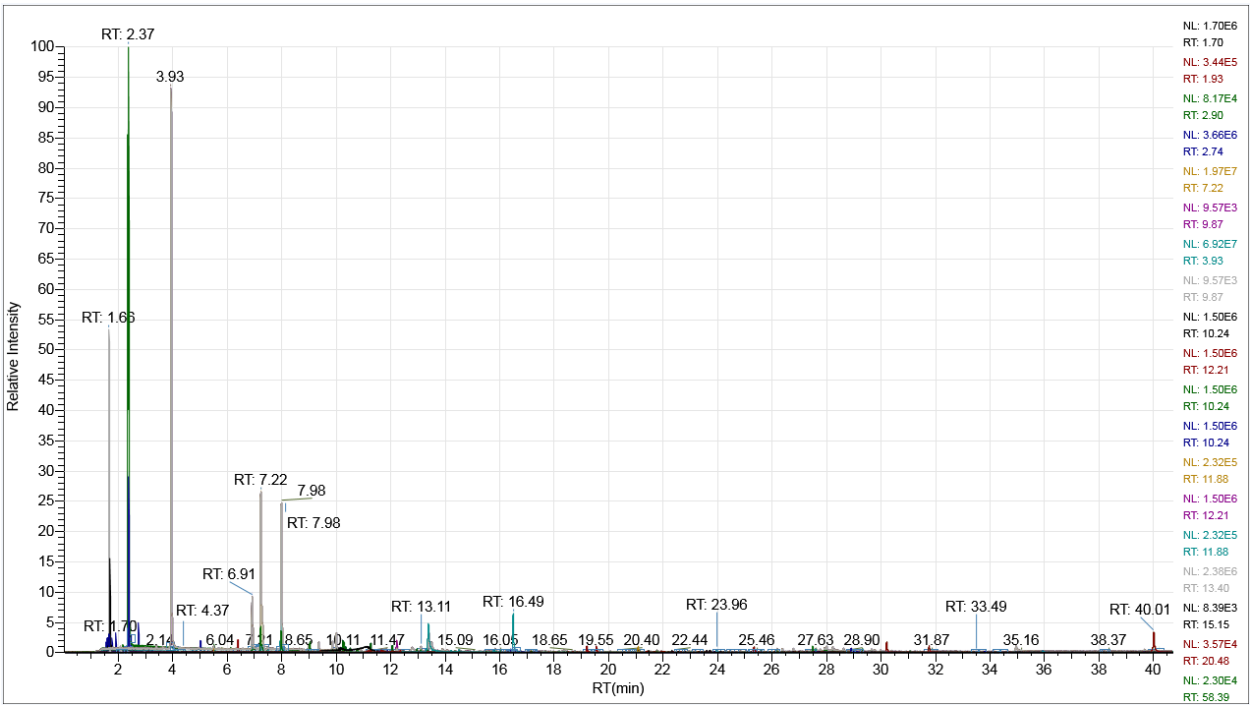

Figure S1. Reconstructed XIC chromatogram of the target analytes in air sample No. 1

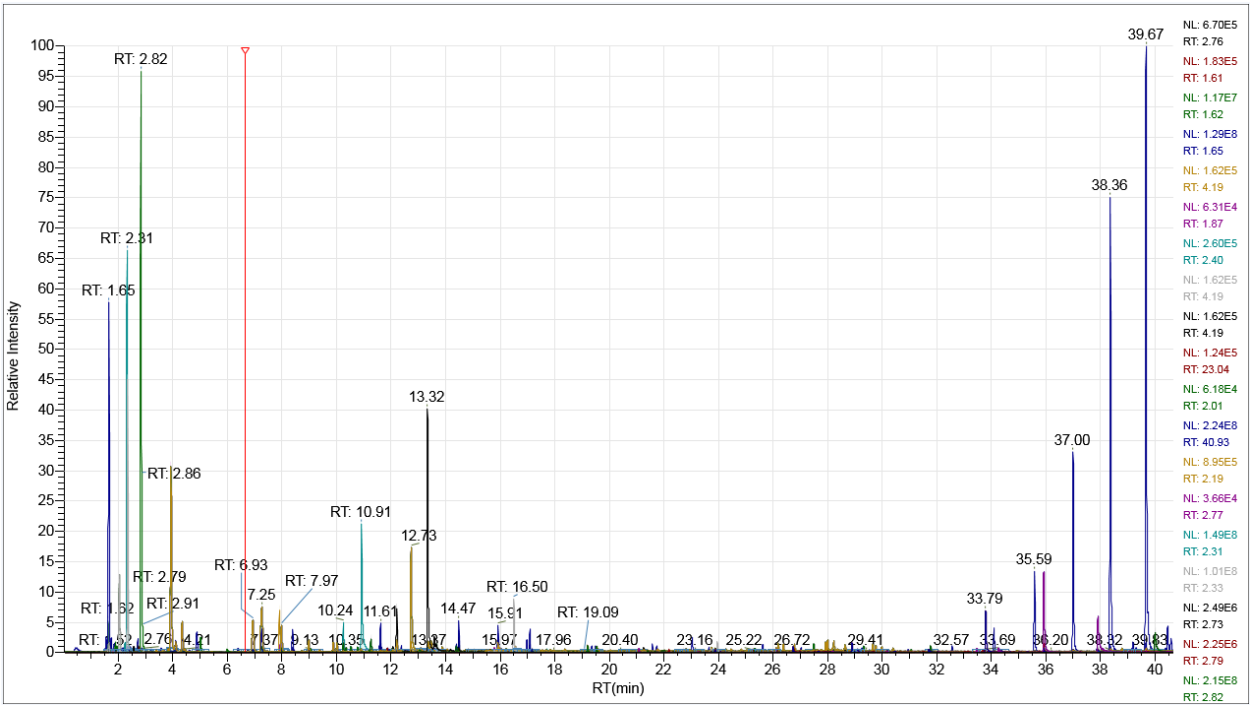

Figure S2. Reconstructed XIC chromatogram of the target analytes in air sample No. 2

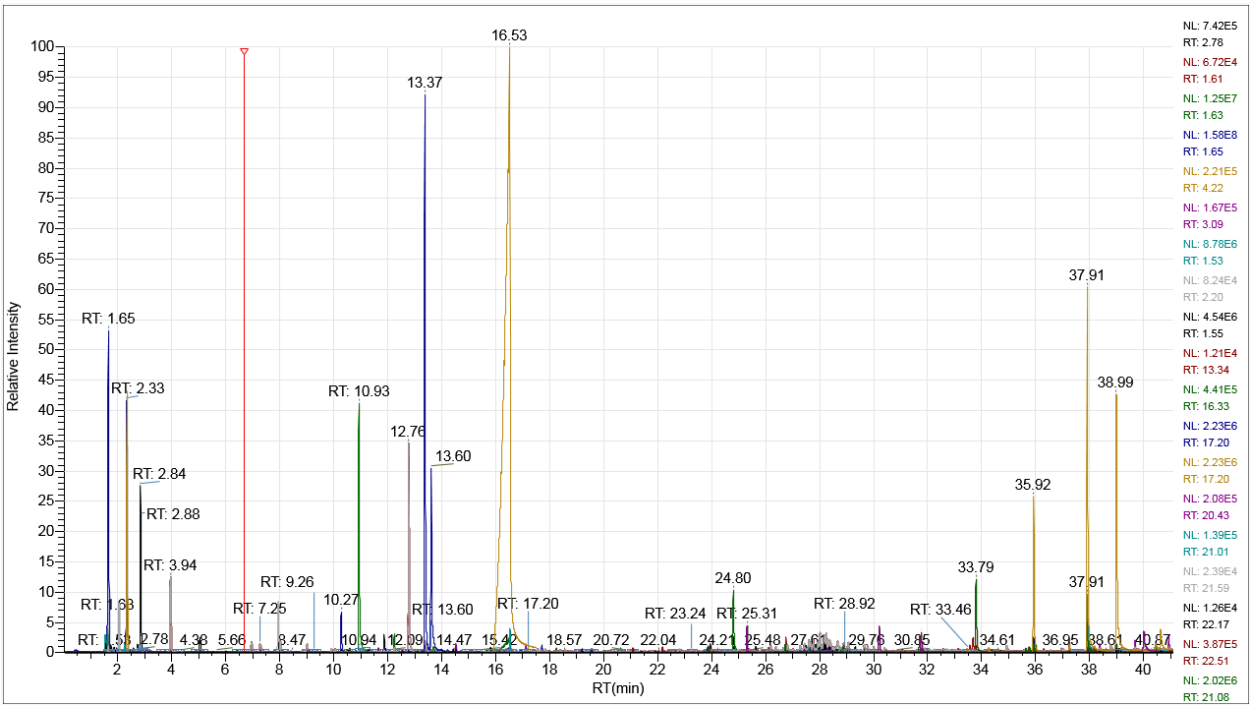

Figure S3. Reconstructed XIC chromatogram of the target analytes in air sample No. 3

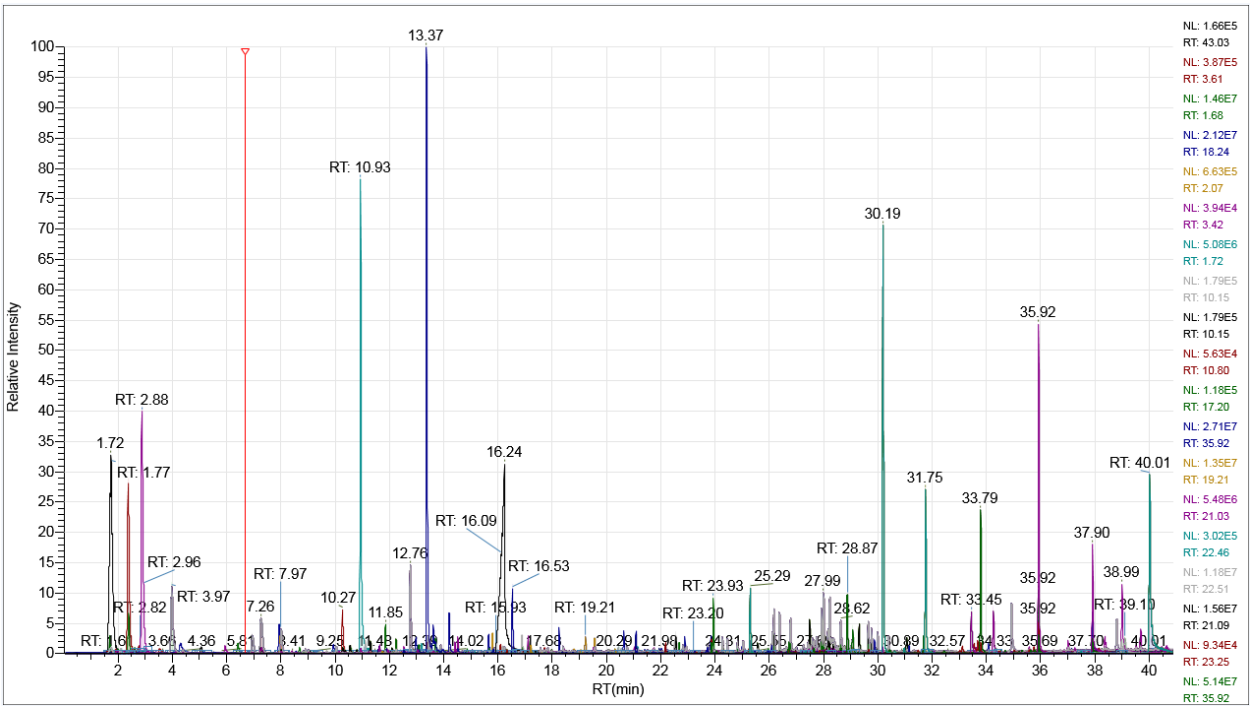

Figure S4. Reconstructed XIC chromatogram of the target analytes in air sample No. 4

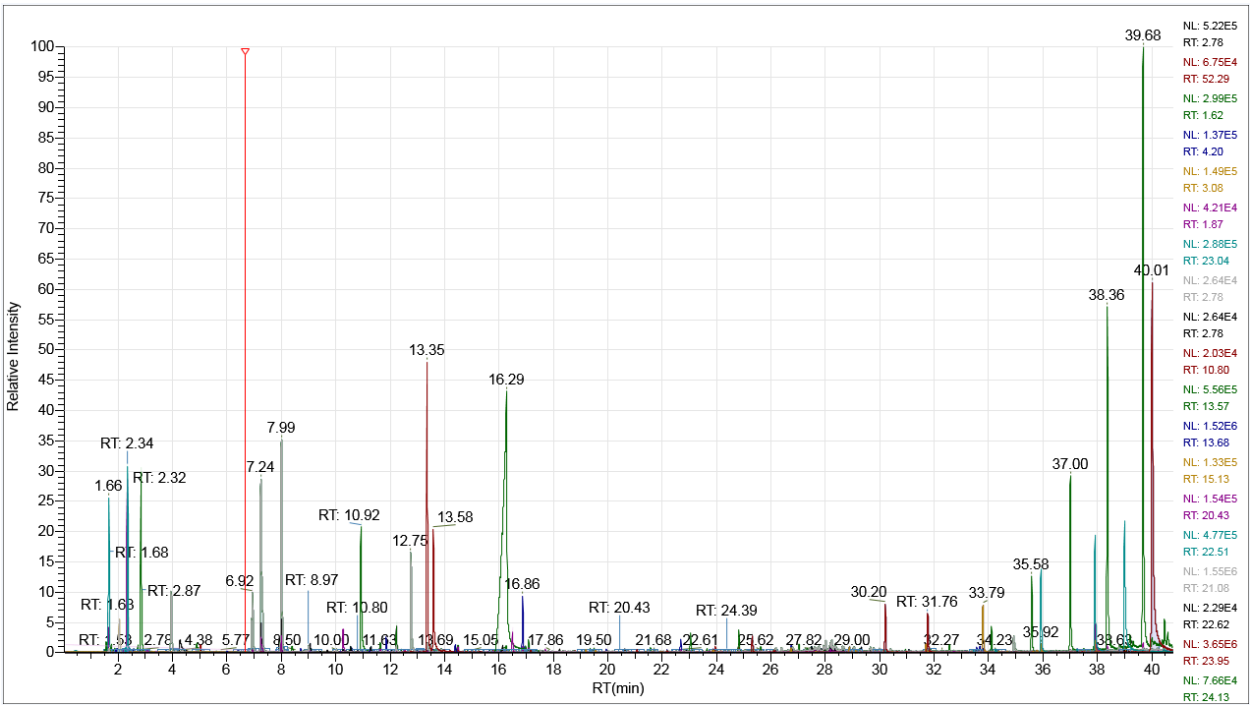

Figure S5. Reconstructed XIC chromatogram of the target analytes in air sample No. 5

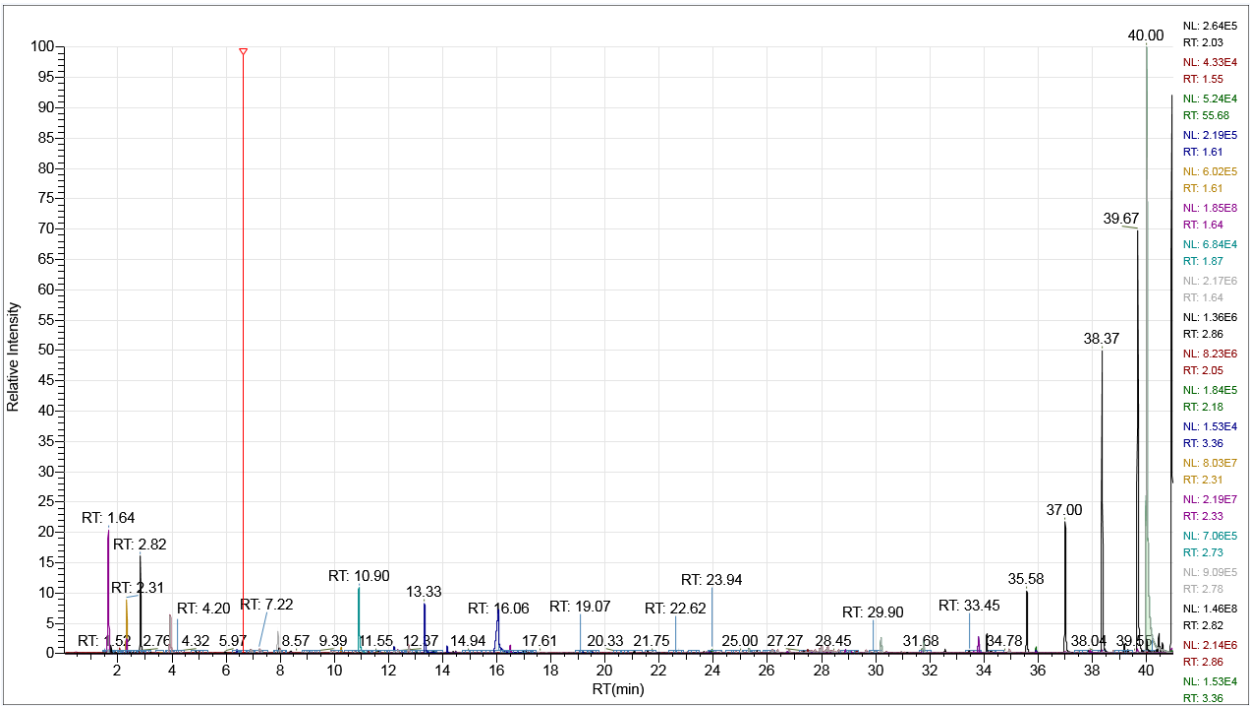

Figure S6. Reconstructed XIC chromatogram of the target analytes in air sample No. 6

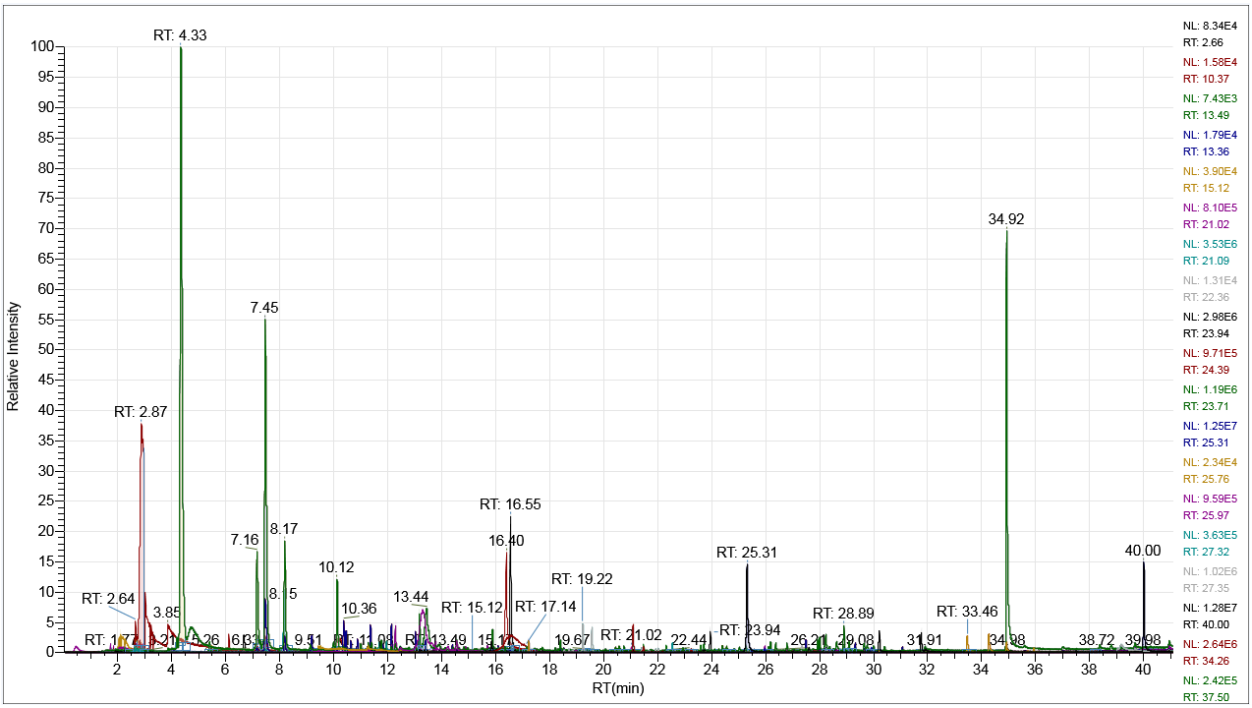

Figure S7. Reconstructed XIC chromatogram of the target analytes in air sample No. 7

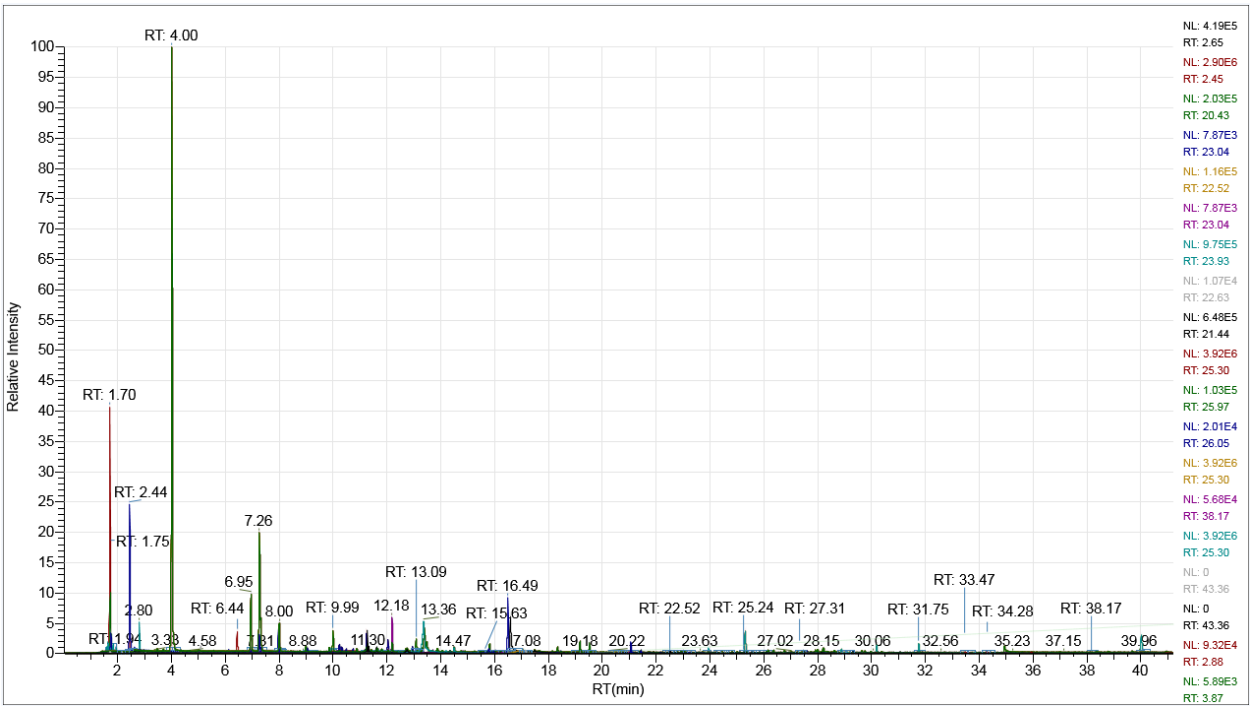

Figure S8. Reconstructed XIC chromatogram of the target analytes in air sample No. 8

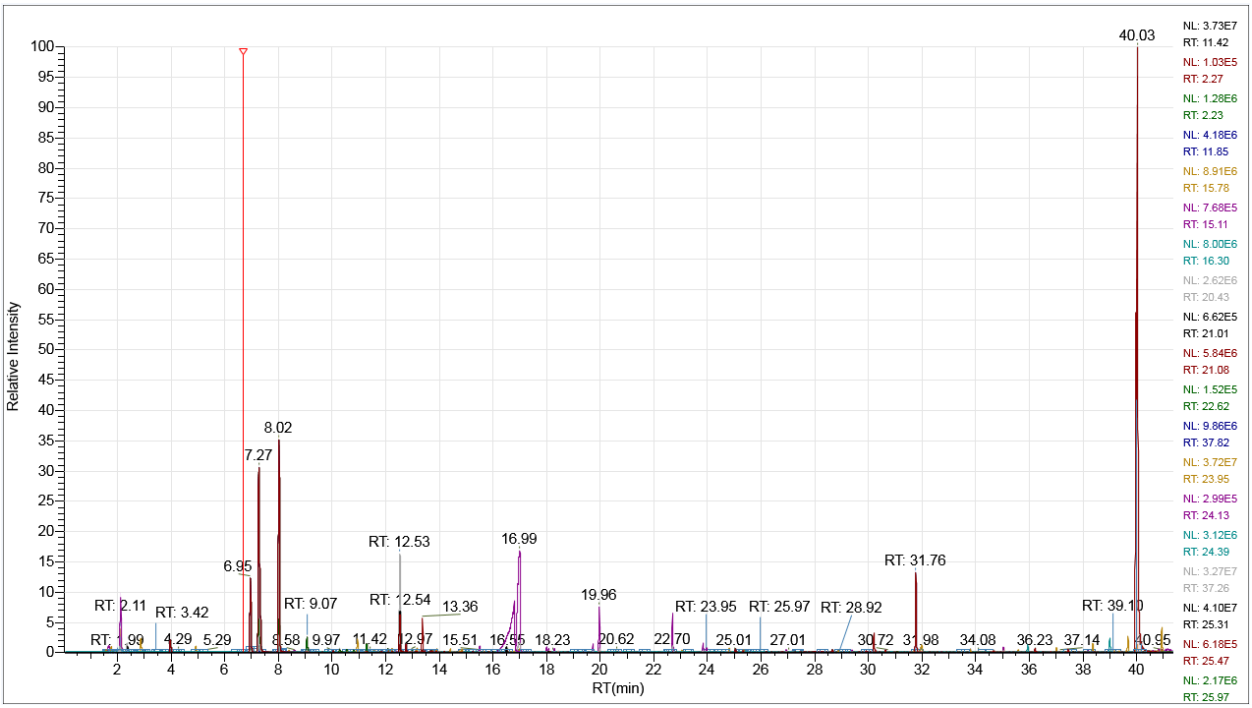

Figure S9. Reconstructed XIC chromatogram of the target analytes in air sample No. 9

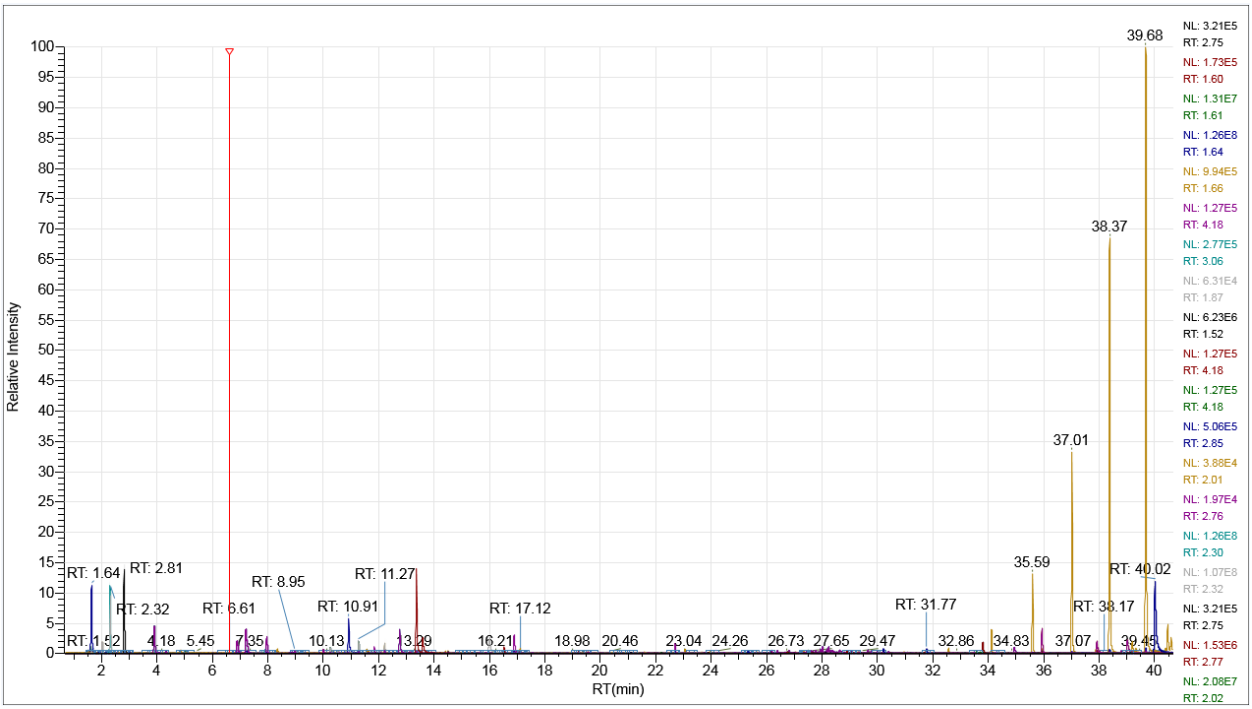

Figure S10. Reconstructed XIC chromatogram of the target analytes in air sample No. 10

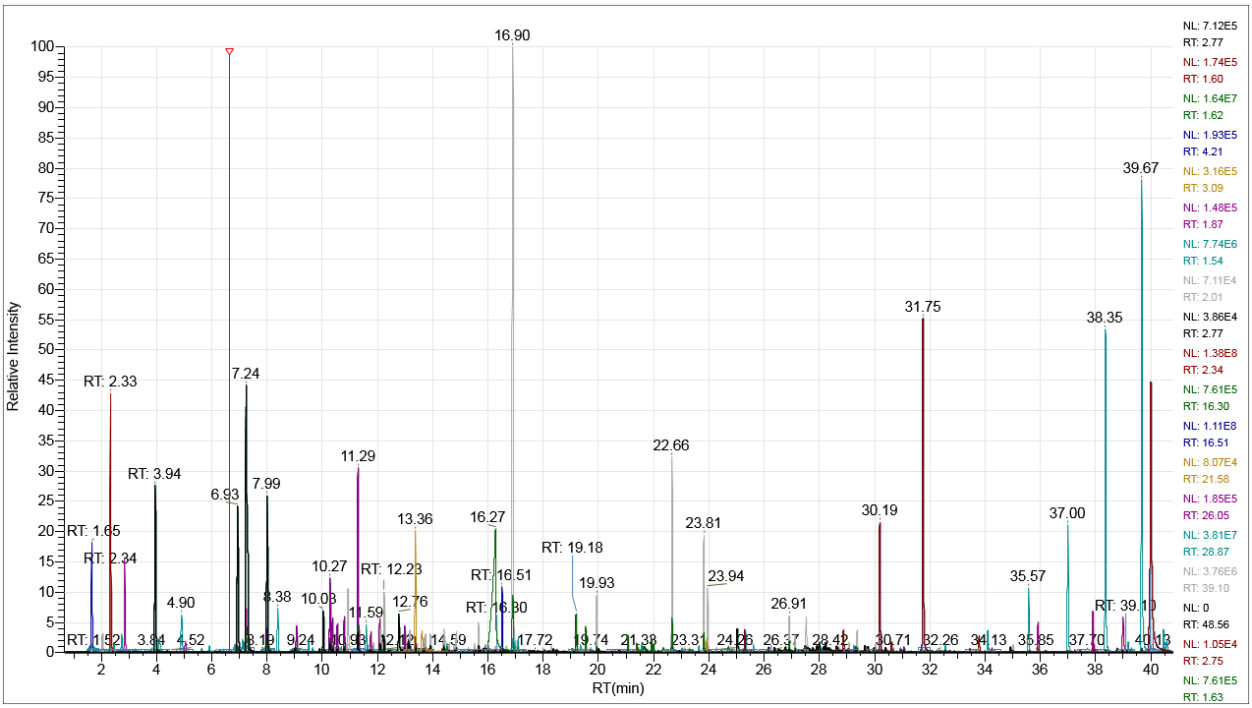

Figure S11. Reconstructed XIC chromatogram of the target analytes in air sample No. 11

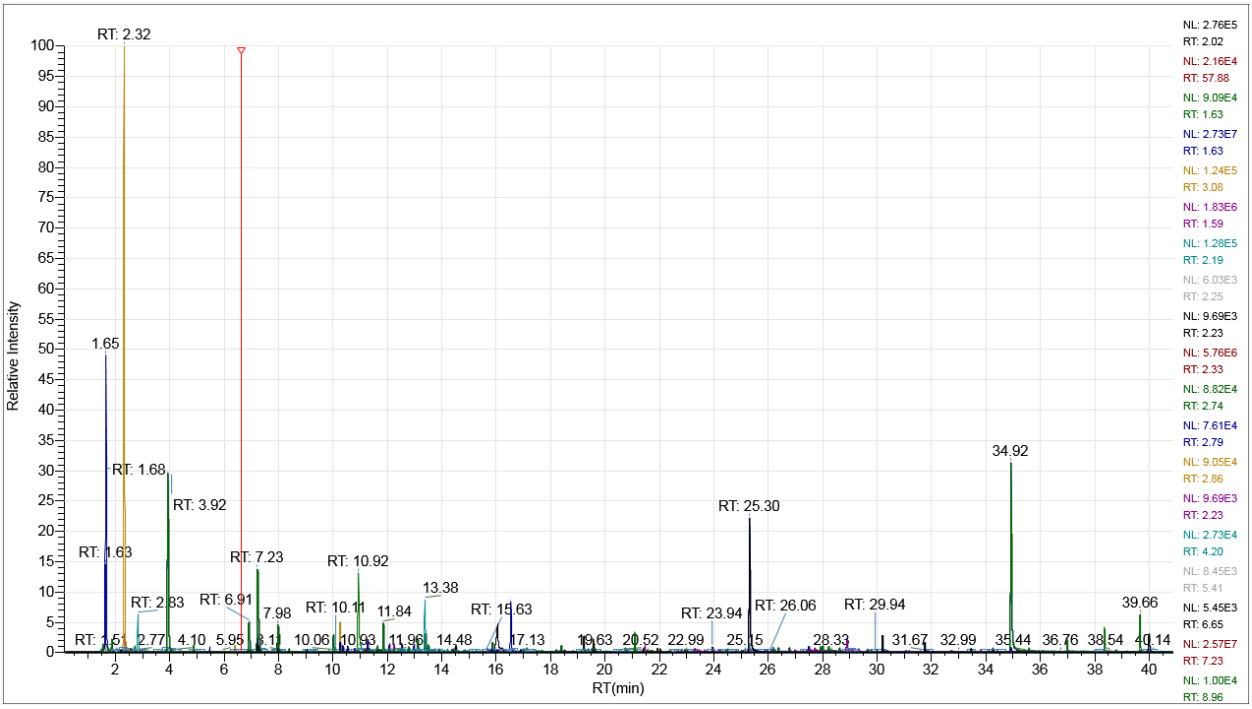

Figure S12. Reconstructed XIC chromatogram of the target analytes in air sample No. 12

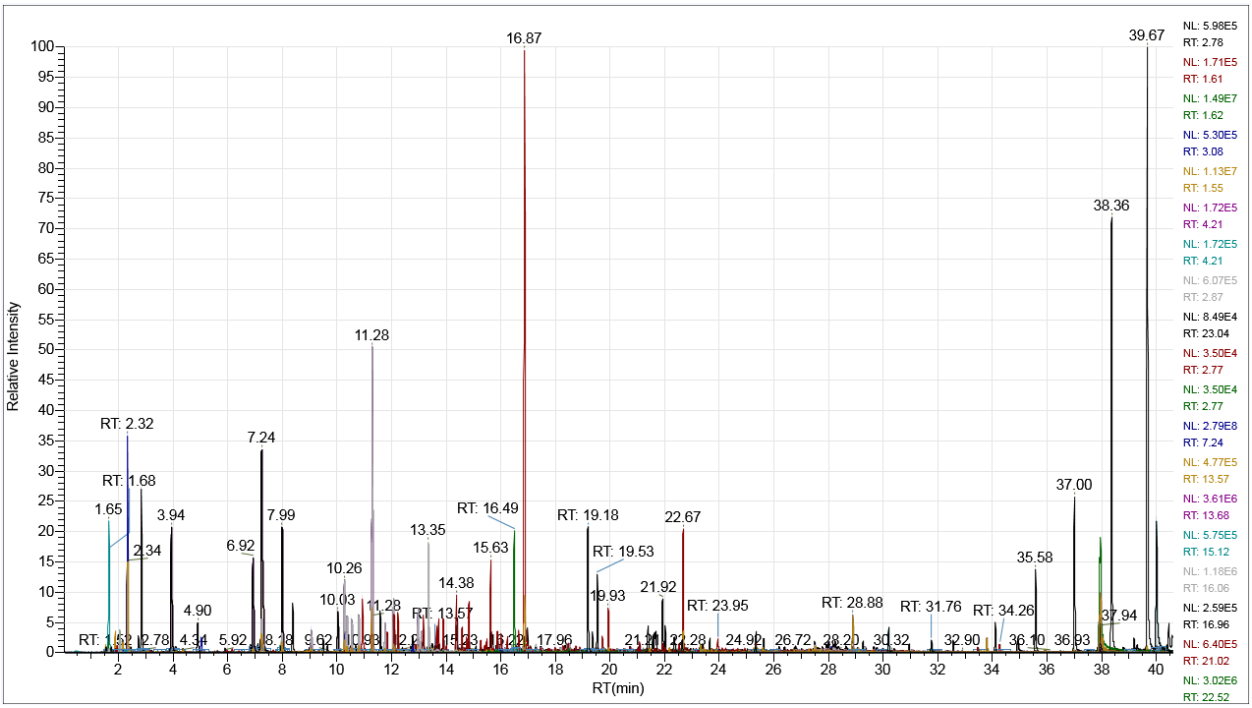

Figure S13. Reconstructed XIC chromatogram of the target analytes in air sample No. 13

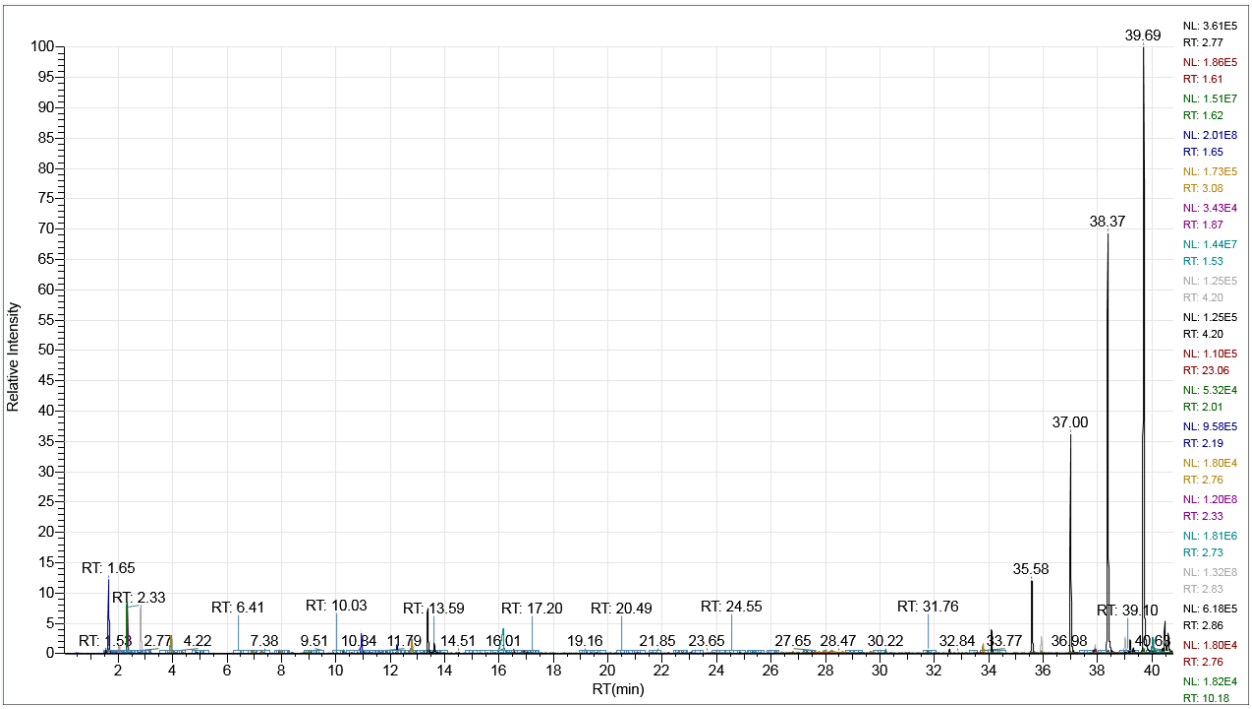

Figure S14. Reconstructed XIC chromatogram of the target analytes in air sample No. 14

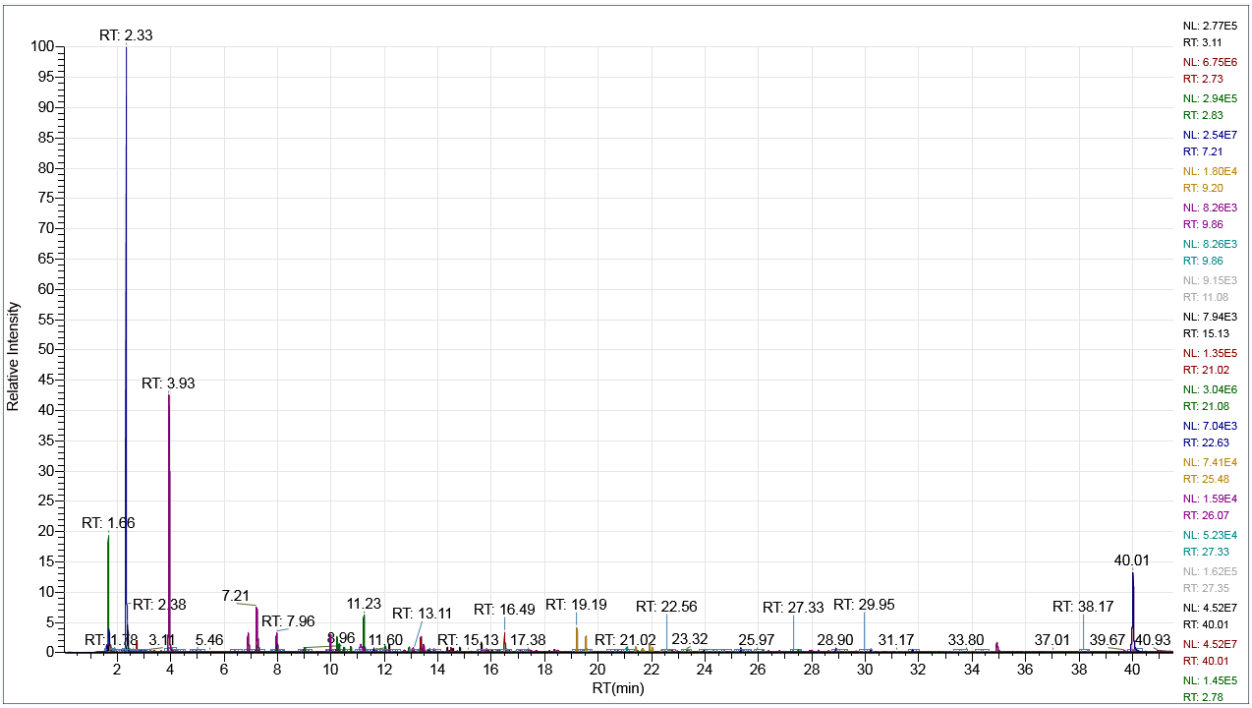

Figure S15. Reconstructed XIC chromatogram of the target analytes in air sample No. 15

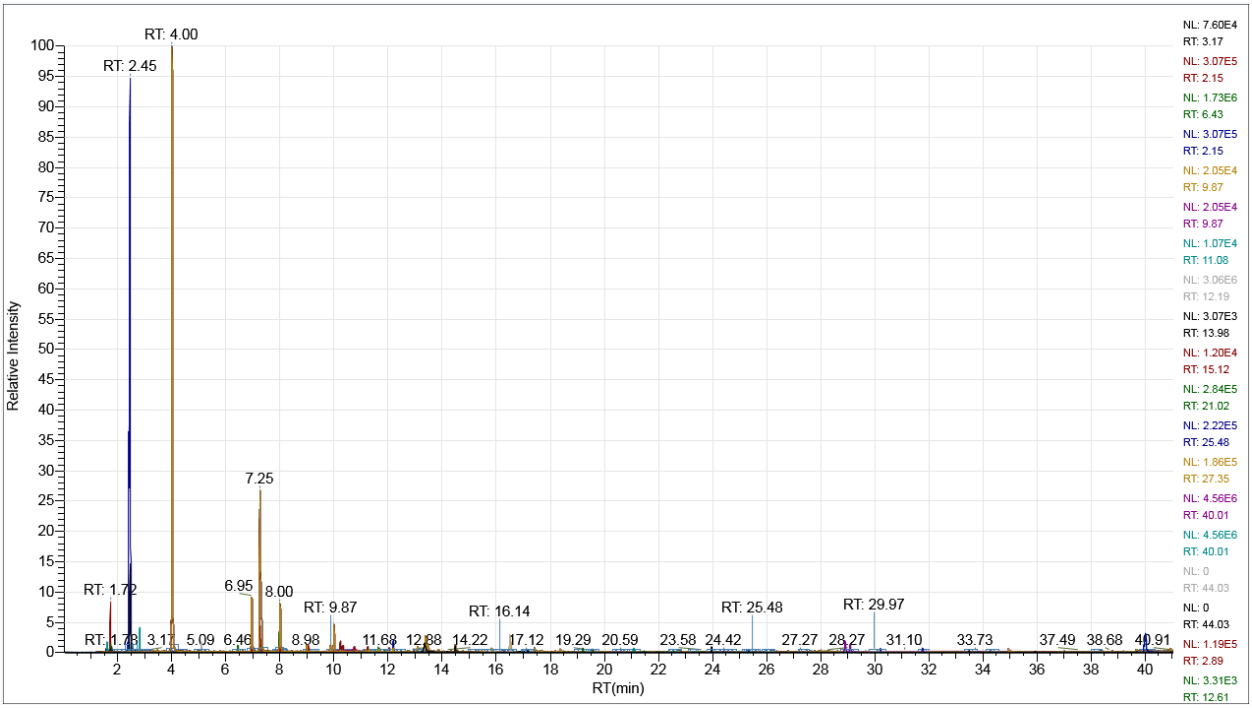

Figure S16. Reconstructed XIC chromatogram of the target analytes in air sample No. 16