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Application Note

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Environment

Analysis of Volatile Hazardous Air Pollutants and Ozone Precursors Using the Cryofocusing GC-MS/MS (MRM) Method

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Environment

1. Introduction

Environmental monitoring of volatile organic compounds in the atmosphere has been carried out for the purposes of understanding the health effects and inferring the sources of photochemical ozone and PM2.5 particulates. Multi-component simultaneous analysis using a canister-based by GC/MS (SIM mode) is widely used as an analytical method for these purposes. 248 substances have been listed as potentially hazardous air pollutants [(1)], and wider application of multi-component simultaneous analysis is being expected.

With the GC/MS (SIM) method, increasing the number of substances subject to measurement can make analysis difficult due to interference among the substances being analyzed or with contaminants.

On the other hand, a multiple reaction monitoring (MRM) method has excellent selectivity and is used as an alternative method to the SIM method, but the number of reports about its application to volatile organic compound analysis is limited [(2)]. In addition, although analytical methods using GCxGC equipment or high-resolution mass spectrometers, such as double focusing and time of flight mass spectrometers, are excellent in terms of selectivity, the application of the GC/MS/MS (MRM) method is considered more practical in the light of the widespread adoption of the equipment.

In this paper, we developed a simultaneous analysis method using a GC/MS/MS (MRM) method for 51 kinds of substances classified as hazardous air pollutants and 55 kinds of photoozone precursors (10 kinds belong to both categories, so 96 kinds) and reported the results of its application to the analysis of environmental samples.

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2. Processes Making up the GC/MS/MS (MRM) Method

2-1. Samples

The standard gas mixture for scan and product ion scan analyses was prepared using 5 mL each of the standard source gases (HAPS-J44+F7 (approximately 1 ppmv each with nitrogen as balance gas [manufactured by Sumitomo Seika]) and PAMS-J58 (approximately 1 ppmv each with nitrogen as balance gas [made by Sumitomo Seika])). A 6-L canister was depressurized using a gas-tight syringe, to which 100 µL of purified water had been added and the standard gas mixture was injected. Then the canister was filled with humidified pure nitrogen gas to 179 kPa (each component at 476 pptv, components duplicated in the two standard source gases at 952 pptv). The standard gas mixture for SIM analysis, MRM analysis and Pseudo-MRM (method where ions with the same mass are selected as precursor ions and product ions) analysis was prepared with each component at 426 pptv and at 852 pptv.

For the internal standard gas, 10 mL of the source gas (1 ppmv each of fluorobenzene, toluene-d8, and chlorobenzene-d5 with nitrogen as balance gas [manufactured by Takachiho Chemical Industrial Co., Ltd.]) was injected into a depressurized 15-L canister, which was then filled up to 250 kPa with humidified pure nitrogen gas (each component at 338 pptv). A canister that had a recovery rate of 90 to 110% for all the components contained in the standard gas described above was used.

General environment atmospheric samples were collected at a residential area of Tokorozawa City, Saitama Prefecture on March 25, 2017 and Sayama City, Saitama Prefecture on March 28. Roadside atmospheric samples were collected at two locations at the side of the national highway in Tokorozawa City, Saitama Prefecture on March 25 and March 28. Samples in the vicinity of sources were collected at two locations on the boundary of an industrial park site in Sayama City, Saitama Prefecture on March 28. Each sample was taken back to the laboratory, its internal pressure was measured after being allowed to return to room temperature, then after pressurizing to 150 kPa with humidified ultra-high purity nitrogen gas, the samples were stored until analysis.

2-2. Equipment and Methods

Fig. 1 shows a GC-MS/MS system equipped with a cryofocusing module.

Tables 1-1 to 1-5 summarize the analysis and SIM measurement conditions, product ion scan analysis conditions, and MRM measurement conditions.

Canister preconcentrator CC2100 Series

GCMS-TQ™8040

Fig. 1 GC-MS/MS System with Canister Preconcentrator

Table 1-1 Analysis Conditions

Canister preconcentrator: CC2100 (GL Sciences)		
Triple quadrupole gas chromatograph mass spectrometer: GCMS-TQ8040 (Shimadzu Corporation)		
Column: InertCap 624, 0.25 mm × 60 m, 1.4 µm (6% Cyano-phenyl / 94% methyl-polysiloxane, GL Sciences, Inc)		
Canister preconcentrator		
Sample transfer flow	:	65 mL/min
Trap temp.	:	Trap 1 (40 °C), Trap 2 (–100 °C)
Dry purge temp.	:	Trap 1 (40 °C), Trap 2 (–20 °C)
Desorb time	:	6 min
Desorb temp.	:	Trap 1 (220 °C), Trap 2 (220 °C)
MCS temp	:	35 °C
Cryo. Cool temp.	:	–185 °C
Inject time	:	2 min
Inject temp.	:	200 °C
Concentration level	:	Internal standard gas (100 mL), standard gas and environmental atmospheric samples (50 to 400 mL)
Carrier gas	:	Helium (1.50 mL/min)
Pressure program	:	Constant flow mode at 155.4 kPa (5 min), 2.41 kPa/min, 172.6 kPa, 4.11 kPa/min, 213.7 kPa, 10.91 kPa/min, 309.2 kPa (2 min)
Gas chromatograph		
Column oven temperature	:	35 °C (5 min), 3.5 °C /min, 60 °C, 6 °C /min, 120 °C, 16 °C /min, 260 °C
Mass spectrometer		
Ion source temperature	:	200 °C
Interface temperature	:	260 °C
Ionization energy	:	70 eV
Collision gas	:	Argon
Set pressure	:	200 kPa

Regarding transitions, the collision energies (CE) of two precursor ions selected based on their intensities in the mass spectra obtained by scan analysis of each compound were measured by product ion scan analysis at 5, 15, 25, 35, 45 V, and two product ions that showed the strongest intensities were selected. By using the selected transitions for these ions, CE was measured in the range 2 to 38 V (with 3 V increments) to determine the optimal CE values. Measurements were made in three modes by changing the mass resolution (Low, Unit, High) and the sensitivity and selectivity were compared.

The elution order of 51 compounds classified as HAPs from the capillary column used (InertCap624) was as described in a previous report [3]. Components listed in PAMS were identified according to NIST library search results by the mass spectrum. Isomers that could not be distinguished in the mass spectrum were identified based on the retention time obtained by scan analysis of the standard gases of the individual isomers prepared by purchasing a standard source gas or authentic preparation (Table 2).

Table 1-2 SIM, Product Ion Scan, MRM, Pseudo-MRM [*1] Methods

Compounds	CAS#	Rt (min)	SIM				
			Target (*m/z*)	Qualifier (*m/z*)	Start time (min)	End time (min)	Event time (sec)
1.1.1.2-Tetrafluoroethane (HFC134a)	811-97-2	4.85	69.0	83.0	4.75	5.35	0.06
n-Propane	115-07-1	4.99	29.0	43.0	4.75	5.35	0.06
Propylene	74-98-6	5.00	41.1	39.0	4.75	5.35	0.06
Dichlorodifluoromethane (CFC12)	75-71-8	5.10	85.0	87.0	4.75	5.35	0.06
Chlorodifluoromethane (HCFC22)	75-45-6	5.14	51.0	67.0	4.75	5.35	0.06
Dichlorotetrafluoroethane (CFC114)	76-14-2	5.53	85.0	135.0	5.35	5.88	0.075
Isobutane	75-28-5	5.58	43.1	57.1	5.35	5.88	0.075
1-Chloro-1,1-difluoroethane (HCFC142b)	75-68-3	5.60	65.0	85.0	5.35	5.88	0.075
Methyl chloride (chloromethane)	74-87-3	5.71	50.0	52.0	5.35	5.88	0.075
1-Butene	106-98-9	6.03	56.1	41.1	5.88	7.00	0.05
n-Butane	106-97-8	6.08	43.1	58.1	5.88	7.00	0.05
Vinyl chloride (chloroethene)	75-01-4	6.09	62.0	64.0	5.88	7.00	0.05
1,3-Butadiene	106-99-0	6.24	54.1	39.1	5.88	7.00	0.05
trans-2-Butene	624-64-6	6.36	41.1	56.1	5.88	7.00	0.05
cis-2-Butene	590-18-1	6.66	41.1	56.1	5.88	7.00	0.05
Methyl bromide (bromomethane)	74-83-9	7.21	93.9	96.0	7.00	7.41	0.3
Ethyl chloride (chloroethane)	75-00-3	7.57	64.0	66.0	7.41	8.09	0.15
Isopentane (2-methylbutane)	78-78-4	7.79	43.1	42.1	7.41	8.09	0.15
Trichlorofluoroethane (CFC11)	75-69-4	8.34	101.0	102.9	8.09	8.84	0.1
1-Pentene	109-67-1	8.44	42.1	55.1	8.09	8.84	0.1
n-Pentane	109-66-0	8.61	43.1	42.1	8.09	8.84	0.1
trans-2-Pentene	646-04-8	9.06	55.1	70.1	8.84	9.71	0.06
1,1-Dichloro-1-fluoroethane (HCFC141b)	1717-00-6	9.22	81.0	83.0	8.84	9.71	0.06
2-Methyl-1,3-butadiene	78-79-5	9.38	67.0	53.0	8.84	9.71	0.06
cis-2-Pentene	627-20-3	9.39	55.1	70.0	8.84	9.71	0.06
2,2-Dichloro-1,1,1-trifluoroethane (HCFC123)	306-83-2	9.48	83.0	85.0	8.84	9.71	0.06
1,1,2-Trifluorotrichloroethane (CFC113)	76-13-1	9.95	101.0	151.0	9.71	10.38	0.1
Vinylidene chloride (1,1-dichloroethylene)	75-35-4	10.00	96.0	61.0	9.71	10.38	0.1
2,2-Dimethylbutane	75-83-2	10.09	43.1	57.1	9.71	10.38	0.1
3,3-Dichloro-1,1,1,2,2-pentafluoropropane (HCFC225ca)	422-56-0	10.74	83.0	85.0	10.38	10.99	0.3
Allyl chloride (3-chloro-1-propene)	107-05-1	11.18	41.1	39.1	10.99	11.99	0.05
1,3-Dichloro-1,1,2,2,3-pentafluoropropane (HCFC225cb)	507-55-1	11.35	67.0	69.0	10.99	11.99	0.05
2,3-Dimethylbutane	79-29-8	11.48	42.1	43.1	10.99	11.99	0.05
2-Methylpentane	107-83-5	11.54	43.1	42.1	10.99	11.99	0.05
Dichloromethane	75-09-2	11.56	49.0	84.0	10.99	11.99	0.05
Cyclopentane	287-92-3	11.76	42.1	55.1	10.99	11.99	0.05
Acrylonitrile	107-13-1	12.17	53.0	52.0	11.99	12.61	0.15
3-Methylpentane	96-14-0	12.34	57.1	56.1	11.99	12.61	0.15
2-Methyl-1-Pentene	763-29-1	12.84	56.1	41.1	12.61	14.17	0.1
n-Hexane	110-54-3	13.13	57.1	41.1	12.61	14.17	0.1
Ethylidene dichloride (1,1-dichloroethane)	75-34-3	13.73	63.0	65.0	12.61	14.17	0.1
2,4-Dimethyl-pentane	108-08-7	14.61	43.1	57.1	14.17	14.82	0.3
Methyl-cyclopentane	96-37-7	15.00	56.1	69.1	14.82	15.69	0.15
cis-1,2-Dichloroethene	156-59-2	15.25	61.0	96.0	14.82	15.69	0.15
Chloroform	67-66-3	16.15	83.0	85.0	15.69	16.35	0.3
2-Methylhexane	591-76-4	16.52	43.1	85.1	16.35	17.31	0.05
Methyl chloroform (1,1,1-trichloroethane)	71-55-6	16.65	97.0	99.0	16.35	17.31	0.05
2,3-Dimethylpentane	565-59-3	16.80	43.1	56.1	16.35	17.31	0.05
Cyclohexane	110-82-7	16.87	84.1	56.1	16.35	17.31	0.05
3-Methylhexane	589-34-4	17.00	43.1	71.1	16.35	17.31	0.05
Carbon Tetrachloride	56-23-5	17.11	116.9	118.9	16.35	17.31	0.05
Benzene	71-43-2	17.58	78.1	77.1	17.31	17.94	0.1
2,2,4-Trimethylpentane	540-84-l	17.66	57.1	56.1	17.31	17.94	0.1
Ethylene dichloride (1,2-dichloroethane)	107-06-2	17.78	62.0	64.0	17.31	17.94	0.1
n-Heptane	142-82-5	18.13	43.1	71.1	17.94	18.75	0.15
Fluorobenzene (IS)	462-6-6	18.31	96.1	70.0	17.94	18.75	0.15
Trichloroethylene	79-01-6	19.24	129.9	131.9	18.75	19.52	0.3
Methylcyclohexane	108-87-2	19.83	83.1	55.1	19.52	20.29	0.15
1,2-Dichloropropane	78-87-5	19.92	63.0	62.0	19.52	20.29	0.15
2,3,4-Trimethylpentane	565-75-3	20.64	43.1	71.1	20.29	21.26	0.15
2-Methylheptane	592-27-8	21.07	57.1	43.1	20.29	21.26	0.15
3-Methylheptane	589-81-1	21.43	43.1	57.1	21.26	22.07	0.15
cis-1,3-Dichloropropene	10061-01-5	21.57	75.0	110.0	21.26	22.07	0.15
Toluene-d8 (IS)	2037-26-5	22.21	98.1	100.1	22.07	23.12	0.075
Toluene	108-88-3	22.39	91.1	92.1	22.07	23.12	0.075
n-Octane	111-65-9	22.50	43.1	85.1	22.07	23.12	0.075
trans-1,3-Dichloropropene	542-75-6	22.89	110.0	75.0	22.07	23.12	0.075
1,1,2-Trichloroethane	79-00-5	23.36	97.0	83.0	23.12	24.08	0.15
Tetrachloroethylene	127-18-4	23.56	165.9	163.9	23.12	24.08	0.15
Ethylene dibromide (1,2-dibromoethane)	106-93-4	24.50	107.0	109.0	24.08	24.87	0.3
Chlorobenzene-d5 (IS)	3114-55-4	25.23	117.1	82.1	24.87	25.89	0.06
Chlorobenzene	108-90-7	25.29	112.0	114.0	24.87	25.89	0.06
Ethylbenzene	100-41-4	25.40	91.1	106.1	24.87	25.89	0.06
n-Nonane	111-84-2	25.51	43.1	57.1	24.87	25.89	0.06

Compounds	CAS#	Rt (min)	SIM				
			Target (*m/z*)	Qualifier (*m/z*)	Start time (min)	End time (min)	Event time (sec)
m-Xylene	108-38-3	25.61	91.1	106.1	24.87	25.89	0.06
p-Xylene	106-42-3	25.61	91.1	106.1	24.87	25.89	0.06
o-Xylene	95-47-6	26.25	91.1	106.1	25.89	27.05	0.1
Styrene	100-42-5	26.30	104.1	78.1	25.89	27.05	0.1
Isopropylbenzene (cumene)	98-82-8	26.81	105.1	120.1	25.89	27.05	0.1
1,1,2,2-Tetrachloroethane	79-34-5	27.25	83.0	85.0	27.05	27.81	0.043
α-Pinene	80-56-8	27.30	93.1	121.1	27.05	27.81	0.043
n-Propylbenzene	103-65-1	27.43	91.1	120.1	27.05	27.81	0.043
3-Ethyltoluene	620-14-4	27.53	105.1	120.1	27.05	27.81	0.043
n-Decane	124-18-5	27.56	57.1	43.1	27.05	27.81	0.043
4-Ethyltoluene	622-96-8	27.61	105.1	120.1	27.05	27.81	0.043
1,3,5-Trimethylbenzene	108-67-8	27.67	105.1	120.1	27.05	27.81	0.043
2-Ethyltoluene	611-14-3	27.95	105.1	120.1	27.81	28.06	0.3
1,2,4-Trimethylbenzene	95-63-6	28.20	105.1	120.1	28.06	28.48	0.1
β-Pinene	127-91-3	28.38	121.1	93.1	28.06	28.48	0.1
m-Dichlorobenzene	541-73-1	28.67	146.0	148.0	28.48	29.03	0.06
1,2,3-Trimethylbenzene	526-73-8	28.76	105.1	120.1	28.48	29.03	0.06
p-Dichlorobenzene	106-46-7	28.82	146.0	148.0	28.48	29.03	0.06
Benzyl chloride	100-44-7	28.92	126.0	91.0	28.48	29.03	0.06
1,3-Diethylbenzene	141-93-5	28.96	105.1	119.1	28.48	29.03	0.06
1,4-Diethylbenzene	105-05-5	29.11	119.1	105.1	29.03	30.28	0.1
n-Undecane	1120-21-4	29.12	57.1	43.1	29.03	30.28	0.1
o-Dichlorobenzene	95-50-1	29.26	146.0	148.0	29.03	30.28	0.1
1,2,4-Trichlorobenzene	120-82-1	31.14	179.9	181.9	30.28	32.00	0.15
Hexachlorobutadiene	87-68-3	31.23	224.9	226.8	30.28	32.00	0.15

*1 Pseudo-MRM is a measurement method where ions with the same mass are selectively measured as precursor ions and product ions. Its advantage in principle is that allows the removal of contaminant ions in the collision cell.

Table 1-3 SIM, Product Ion Scan, MRM, Pseudo-MRM [*1] Methods

Compounds	CAS#	Rt (min)	Product Ion Scan								
			Start time (min)	End time (min)	Event time (sec)	Start (*m/z*)	End (*m/z*)	Precursor (*m/z*)	Start (*m/z*)	End (*m/z*)	Precursor (*m/z*)
1.1.1.2-Tetrafluoroethane (HFC134a)	811-97-2	4.85	3.50	4.97	0.15	29	84	69	29	98	83
n-Propane	115-07-1	4.99	4.49	5.31	0.075	15	44	29	15	58	43
Propylene	74-98-6	5.00	4.49	5.31	0.075	15	56.1	41.1	15	54	39
Dichlorodifluoromethane (CFC12)	75-71-8	5.10	4.97	5.28	0.075	29	100	85	29	102	87
Chlorodifluoromethane (HCFC22)	75-45-6	5.14	4.97	5.28	0.075	29	66	51	29	82	67
Dichlorotetrafluoroethane (CFC114)	76-14-2	5.53	5.28	5.91	0.05	29	100	85	29	150	135
Isobutane	75-28-5	5.58	5.31	5.85	0.15	15	58.1	43.1	15	72.1	57.1
1-Chloro-1,1-difluoroethane (HCFC142b)	75-68-3	5.60	5.28	5.91	0.05	29	80	65	29	100	85
Methyl chloride (chloromethane)	74-87-3	5.71	5.28	5.91	0.05	29	65	50	29	67	52
1-Butene	106-98-9	6.03	5.85	6.22	0.075	15	71.1	56.1	15	56.1	41.1
n-Butane	106-97-8	6.08	5.85	6.22	0.075	15	58.1	43.1	15	73.1	58.1
Vinyl chloride (chloroethene)	75-01-4	6.09	5.91	6.71	0.075	29	77	62	29	79	64
1,3-Butadiene	106-99-0	6.24	5.91	6.71	0.075	29	69.1	54.1	29	54.1	39.1
trans-2-Butene	624-64-6	6.36	6.22	6.52	0.15	15	56.1	41.1	15	71.1	56.1
cis-2-Butene	590-18-1	6.66	6.52	7.22	0.15	15	56.1	41.1	15	71.1	56.1
Methyl bromide (bromomethane)	74-83-9	7.21	6.71	7.40	0.15	29	108.9	93.9	29	111	96
Ethyl chloride (chloroethane)	75-00-3	7.57	7.40	8.75	0.075	29	79	64	29	81	66
Isopentane (2-methylbutane)	78-78-4	7.79	7.22	8.00	0.15	15	58.1	43.1	15	57.1	42.1
Trichlorofluoroethane (CFC11)	75-69-4	8.34	7.40	8.75	0.075	29	116	101	29	117.9	102.9
1-Pentene	109-67-1	8.44	8.00	8.77	0.075	15	57.1	42.1	15	70.1	55.1
n-Pentane	109-66-0	8.61	8.00	8.77	0.075	15	58.1	43.1	15	57.1	42.1
trans-2-Pentene	646-04-8	9.06	8.77	9.18	0.15	15	70.1	55.1	15	85.1	70.1
1,1-Dichloro-1-fluoroethane (HCFC141b)	1717-00-6	9.22	8.75	9.73	0.075	29	96	81	29	98	83
2-Methyl-1,3-butadiene	78-79-5	9.38	9.18	9.63	0.05	15	68	53	15	82	67
cis-2-Pentene	627-20-3	9.39	9.18	9.63	0.05	15	70.1	55.1	15	85.1	70.1
2,2-Dichloro-1,1,1-trifluoroethane (HCFC123)	306-83-2	9.48	8.75	9.73	0.075	29	98	83	29	100	85
1,1,2-Trifluorotrichloroethane (CFC113)	76-13-1	9.95	9.73	10.35	0.075	29	116	101	29	166	151
Vinylidene chloride (1,1-dichloroethylene)	75-35-4	10.00	9.73	10.35	0.075	29	111	96	29	76	61
2,2-Dimethylbutane	75-83-2	10.09	9.63	10.78	0.15	15	86.2	71.2	15	72.1	57.1
3,3-Dichloro-1,1,1,2,2-pentafluoropropane (HCFC225ca)	422-56-0	10.74	10.35	10.98	0.15	29	98	83	29	100	85
Allyl chloride (3-chloro-1-propene)	107-05-1	11.18	10.98	11.86	0.05	29	56.1	41.1	29	54.1	39.1
1,3-Dichloro-1,1,2,2,3-pentafluoropropane (HCFC225cb)	507-55-1	11.35	10.98	11.86	0.05	29	82	67	29	84	69
2,3-Dimethylbutane	79-29-8	11.48	10.78	11.99	0.05	15	57.1	42.1	15	58.1	43.1
2-Methylpentane	107-83-5	11.54	10.78	11.99	0.05	15	58.1	43.1	29	86.1	71.1
Dichloromethane	75-09-2	11.56	10.98	11.86	0.05	29	64	49	29	99	84
Cyclopentane	287-92-3	11.76	10.78	11.99	0.05	15	70.1	55.1	15	70.1	70.1
Acrylonitrile	107-13-1	12.17	11.86	13.00	0.15	29	68	53	29	67	52

Compounds	CAS#	Rt (min)	Product Ion Scan								
			Start time (min)	End time (min)	Event time (sec)	Start (*m/z*)	End (*m/z*)	Precursor (*m/z*)	Start (*m/z*)	End (*m/z*)	Precursor (*m/z*)
3-Methylpentane	96-14-0	12.34	11.99	12.52	0.15	15	72.1	57.1	15	71.1	56.1
2-Methyl-1-Pentene	763-29-1	12.84	12.52	12.92	0.15	15	71.1	56.1	15	56.1	69.1
n-Hexane	110-54-3	13.13	12.92	13.86	0.15	15	72.1	57.1	15	56.1	86.1
Ethylidene dichloride (1,1-dichloroethane)	75-34-3	13.73	13.00	14.47	0.15	29	78	63	29	80	65
2,4-Dimethyl-pentane	108-08-7	14.61	13.86	14.76	0.15	15	58.1	43.1	15	72.1	57.1
Methyl-cyclopentane	96-37-7	15.00	14.76	15.76	0.15	15	71.1	56.1	15	84.1	69.1
cis-1,2-Dichloroethene	156-59-2	15.25	14.47	15.69	0.15	29	76	61	29	111	96
Chloroform	67-66-3	16.15	15.69	16.40	0.15	29	98	83	29	100	85
2-Methylhexane	591-76-4	16.52	15.76	17.24	0.038	15	58.1	43.1	15	100.1	85.1
Methyl chloroform (1,1,1-trichloroethane)	71-55-6	16.65	16.40	16.88	0.15	29	112	97	29	114	99
2,3-Dimethylpentane	565-59-3	16.80	15.76	17.24	0.038	15	58.1	43.1	15	71.1	56.1
Cyclohexane	110-82-7	16.87	15.76	17.24	0.038	15	99.1	84.1	15	71.1	56.1
3-Methylhexane	589-34-4	17.00	15.76	17.24	0.038	15	58.1	43.1	15	58.1	56.1
Carbon Tetrachloride	56-23-5	17.11	16.88	17.33	0.15	29	131.9	116.9	29	133.9	118.9
Benzene	71-43-2	17.58	17.33	18.12	0.075	29	93.1	78.1	29	92.1	77.1
2,2,4-Trimethylpentane	540-84-l	17.66	17.24	17.85	0.075	15	72.1	57.1	15	71.1	56.1
Ethylene dichloride (1,2-dichloroethane)	107-06-2	17.78	17.33	18.12	0.075	29	77	62	29	79	64
n-Heptane	142-82-5	18.13	17.85	19.07	0.075	15	58.1	43.1	15	86.1	71.1
Fluorobenzene (IS)	462-6-6	18.31	17.85	19.07	0.075	15	111.1	96.1	15	85	70
Trichloroethylene	79-01-6	19.24	18.12	19.58	0.075	29	144.9	129.9	29	146.9	131.9
Methylcyclohexane	108-87-2	19.83	19.07	20.24	0.15	15	98.1	83.1	15	98.1	98.1
1,2-Dichloropropane	78-87-5	19.92	19.58	20.75	0.15	29	78	63	29	77	62
2,3,4-Trimethylpentane	565-75-3	20.64	20.24	20.79	0.15	15	58.1	43.1	15	86.1	71.1
2-Methylheptane	592-27-8	21.07	20.79	21.21	0.15	15	72.1	99.1	15	72.1	57.1
3-Methylheptane	589-81-1	21.43	21.21	21.80	0.15	15	58.1	43.1	15	72.1	57.1
cis-1,3-Dichloropropene	10061-01-5	21.57	20.75	21.98	0.15	29	90	75	29	125	110
Toluene-d8 (IS)	2037-26-5	22.21	21.80	24.82	0.05	15	113.1	98.1	15	115.1	100.1
Toluene	108-88-3	22.39	21.98	22.68	0.075	29	106.1	91.1	29	107.1	92.1
n-Octane	111-65-9	22.50	21.80	24.82	0.05	15	100.1	85.1	15	58.1	43.1
trans-1,3-Dichloropropene	542-75-6	22.89	22.68	23.12	0.15	29	125	110	29	90	75
1,1,2-Trichloroethane	79-00-5	23.36	23.12	23.46	0.15	29	112	97	29	98	83
Tetrachloroethylene	127-18-4	23.56	23.46	24.02	0.15	29	180.9	165.9	29	178.9	163.9
Ethylene dibromide (1,2-dibromoethane)	106-93-4	24.50	24.02	24.92	0.15	29	122	107	29	124	109
Chlorobenzene-d5 (IS)	3114-55-4	25.23	24.82	25.94	0.038	15	132.1	117.1	15	97.1	82.1
Chlorobenzene	108-90-7	25.29	24.92	25.49	0.05	29	127	112	29	129	114
Ethylbenzene	100-41-4	25.40	24.92	25.49	0.05	29	106.1	91.1	29	121.1	106.1
n-Nonane	111-84-2	25.51	24.82	25.94	0.038	15	58.1	43.1	15	72.1	57.1
m-Xylene	108-38-3	25.61	25.49	25.95	0.15	29	106.1	91.1	29	121.1	106.1
p-Xylene	106-42-3	25.61	24.82	25.94	0.038	15	106.1	91.1	15	121.1	106.1
o-Xylene	95-47-6	26.25	25.95	26.74	0.075	29	106.1	91.1	29	121.1	106.1
Styrene	100-42-5	26.30	25.95	26.74	0.075	29	119.1	104.1	29	93.1	78.1
Isopropylbenzene (cumene)	98-82-8	26.81	26.49	27.02	0.15	15	120.1	105.1	15	135.1	120.1
1,1,2,2-Tetrachloroethane	79-34-5	27.25	26.74	27.43	0.15	29	98	83	29	100	85
α-Pinene	80-56-8	27.30	27.02	27.31	0.15	15	108.1	93.1	15	136.1	121.1
n-Propylbenzene	103-65-1	27.43	27.31	27.75	0.03	15	106.1	91.1	15	135.1	120.1
3-Ethyltoluene	620-14-4	27.53	27.31	27.75	0.03	15	120.1	105.1			
n-Decane	124-18-5	27.56	27.31	27.75	0.03	15	72.1	57.1	15	58.1	43.1
4-Ethyltoluene	622-96-8	27.61	27.43	27.94	0.075	29	120.1	105.1	29	135.1	120.1
1,3,5-Trimethylbenzene	108-67-8	27.67	27.43	27.94	0.075	29	120.1	105.1	29	135.1	120.1
2-Ethyltoluene	611-14-3	27.95	27.75	28.05	0.15	15	120.1	105.1	15	135.1	120.1
1,2,4-Trimethylbenzene	95-63-6	28.20	27.94	28.45	0.15	29	120.1	105.1	29	135.1	120.1
β-Pinene	127-91-3	28.38	28.05	28.47	0.05	15	136.1	121.1	15	108.1	93.1
m-Dichlorobenzene	541-73-1	28.67	28.45	28.76	0.15	29	161	146	29	163	148
1,2,3-Trimethylbenzene	526-73-8	28.76	28.47	28.85	0.15	15	120.1	105.1	15	135.1	120.1
p-Dichlorobenzene	106-46-7	28.82	28.76	29.10	0.075	29	161	146	29	163	148
Benzyl chloride	100-44-7	28.92	28.76	29.10	0.075	29	141	126	29	106	91
1,3-Diethylbenzene	141-93-5	28.96	28.85	29.02	0.15	15	120.1	105.1	15	134.1	119.1
1,4-Diethylbenzene	105-05-5	29.11	29.02	32.00	0.075	15	134.1	119.1	15	120.1	105.1
n-Undecane	1120-21-4	29.12	29.02	32.00	0.075	15	72.1	57.1	15	58.1	43.1
o-Dichlorobenzene	95-50-1	29.26	29.10	30.02	0.15	29	161	146	29	163	148
1,2,4-Trichlorobenzene	120-82-1	31.14	30.02	31.55	0.075	29	194.9	179.9	29	196.9	181.9
Hexachlorobutadiene	87-68-3	31.23	30.02	31.55	0.075	29	239.9	224.9	29	241.8	226.8

*1 Pseudo-MRM is a measurement method where ions with the same mass are selectively measured as precursor ions and product ions. Its advantage in principle is that allows the removal of contaminant ions in the collision cell.

Table 1-4 SIM, Product Ion Scan, MRM, Pseudo-MRM [*1] Methods

Compounds	CAS#	Rt (min)	MRM						
			Start time (min)	End (min)	Event (sec)	Target transition (*m/z*)	CE (V)	Qualifoer transition (*m/z*)	CE (V)
1.1.1.2-Tetrafluoroethane (HFC134a)	811-97-2	4.85	4.35	5.38	0.06	83.0>33.0	11	69.0>50.0	26
n-Propane	115-07-1	4.99	4.35	5.38	0.06	29.1>27.1	2	43.1>27.1	11
Propylene	74-98-6	5.00	4.35	5.38	0.06	41.1>39.0	6	29.1>15.0	27
Dichlorodifluoromethane (CFC12)	75-71-8	5.10	4.35	5.38	0.06	85.0>50.0	25	87.0>50.0	25
Chlorodifluoromethane (HCFC22)	75-45-6	5.14	4.35	5.38	0.06	51.0>31.0	23	67.0>31.0	20
Dichlorotetrafluoroethane (CFC114)	76-14-2	5.53	5.38	5.83	0.075	135.0>85.0	11	85.0>50.0	25
Isobutane	75-28-5	5.58	5.38	5.83	0.075	43.1>27.1	9	57.1>29.0	9
1-Chloro-1,1-difluoroethane (HCFC142b)	75-68-3	5.60	5.38	5.83	0.075	65.0>45.0	17	85.0>50.0	25
Methyl chloride (chloromethane)	74-87-3	5.71	5.38	5.83	0.075	50.0>15.0	11	52.0>15.0	11
1-Butene	106-98-9	6.03	5.83	6.95	0.05	41.1>39.0	6	56.1>41.1	9
n-Butane	106-97-8	6.08	5.83	6.95	0.05	43.1>27.1	9	58.1>43.10	2
Vinyl chloride (chloroethene)	75-01-4	6.09	5.83	6.95	0.05	62.0>27.1	11	64.0>27.1	11
1,3-Butadiene	106-99-0	6.24	5.83	6.95	0.05	54.0>39.0	10	54.0>28.0	11
trans-2-Butene	624-64-6	6.36	5.83	6.95	0.05	41.1>39.1	6	56.1>41.1	9
cis-2-Butene	590-18-1	6.66	5.83	6.95	0.05	41.1>39.1	5	56.1>41.1	9
Methyl bromide (bromomethane)	74-83-9	7.21	6.95	7.40	0.3	94.0>15.0	17	96.0>15.0	17
Ethyl chloride (chloroethane)	75-00-3	7.57	7.40	8.06	0.15	64.0>29.0	5	64.0>49.0	17
Isopentane (2-methylbutane)	78-78-4	7.79	7.40	8.06	0.15	57.1>29.1	9	43.1>27.1	9
Trichlorofluoroethane (CFC11)	75-69-4	8.34	8.06	8.80	0.1	101.0>66.0	26	103.0>66.0	26
1-Pentene	109-67-1	8.44	8.06	8.80	0.1	70.1>55.0	7	42.1>27.1	15
n-Pentane	109-66-0	8.61	8.06	8.80	0.1	42.1>27.1	15	43.1>27.1	9
trans-2-Pentene	646-04-8	9.06	8.80	9.71	0.06	70.1>55.1	9	55.1>29.1	9
1,1-Dichloro-1-fluoroethane (HCFC141b)	1717-00-6	9.22	8.80	9.71	0.06	81.0>61.0	14	83.0>63.0	14
2-Methyl-1,3-butadiene	78-79-5	9.38	8.80	9.71	0.06	70.1>55.1	9	55.1>27.1	15
cis-2-Pentene	627-20-3	9.39	8.80	9.71	0.06	67.0>41.0	15	53.1>27.1	9
2,2-Dichloro-1,1,1-trifluoroethane (HCFC123)	306-83-2	9.48	8.80	9.71	0.06	83.0>47.0	26	85.0>47.0	26
1,1,2-Trifluorotrichloroethane (CFC113)	76-13-1	9.95	9.71	10.45	0.1	151.0>101.0	11	101.0>66.0	26
Vinylidene chloride (1,1-dichloroethylene)	75-35-4	10.00	9.71	10.45	0.1	96.0>61.0	17	61.0>26.0	21
2,2-Dimethylbutane	75-83-2	10.09	9.71	10.45	0.1	57.1>29.1	9	71.1>29.1	18
3,3-Dichloro-1,1,1,2,2-pentafluoropropane (HCFC225ca)	422-56-0	10.74	10.45	10.98	0.3	83.0>45.0	24	85.0>49.0	26
Allyl chloride (3-chloro-1-propene)	107-05-1	11.18	10.98	11.98	0.05	76.0>41.0	8	76.0>39.0	8
1,3-Dichloro-1,1,2,2,3-pentafluoropropane (HCFC225cb)	507-55-1	11.35	10.98	11.98	0.05	67.0>31.0	25	85.0>50.0	26
2,3-Dimethylbutane	79-29-8	11.48	10.98	11.98	0.05	42.1>27.1	17	43.1>15.1	22
2-Methylpentane	107-83-5	11.54	10.98	11.98	0.05	43.1>27.1	10	71.1>41.1	7
Dichloromethane	75-09-2	11.56	10.98	11.98	0.05	84.0>49.0	8	86.0>51.0	8
Cyclopentane	287-92-3	11.76	10.98	11.98	0.05	70.1>55.1	18	42.1>27.1	6
Acrylonitrile	107-13-1	12.17	11.98	12.57	0.15	53.0>26.0	8	52.0>26.0	8
3-Methylpentane	96-14-0	12.34	11.98	12.57	0.15	56.1>41.1	9	57.1>29.1	9
2-Methyl-1-Pentene	763-29-1	12.84	12.57	13.43	0.15	56.1>41.1	9	84.1>56.1	6
n-Hexane	110-54-3	13.13	12.57	13.43	0.15	57.1>29.1	9	86.1>41.1	15
Ethylidene dichloride (1,1-dichloroethane)	75-34-3	13.73	13.43	14.18	0.3	63.0>27.0	17	65.0>27.0	17
2,4-Dimethyl-pentane	108-08-7	14.61	14.18	14.77	0.3	57.1>29.1	9	85.1>43.1	7
Methyl-cyclopentane	96-37-7	15.00	14.77	15.69	0.15	56.1>41.0	9	69.1>41.1	9
cis-1,2-Dichloroethene	156-59-2	15.25	14.77	15.69	0.15	96.0>61.0	17	61.0>26.0	22
Chloroform	67-66-3	16.15	15.69	16.30	0.3	83.0>47.0	26	85.0>47.0	26
2-Methylhexane	591-76-4	16.52	16.30	17.30	0.05	85.1>43.1	9	43.1>27.1	9
Methyl chloroform (1,1,1-trichloroethane)	71-55-6	16.65	16.30	17.30	0.05	97.0>61.0	17	99.0>61.0	17
2,3-Dimethylpentane	565-59-3	16.80	16.30	17.30	0.05	56.1>41.1	9	71.1>43.1	6
Cyclohexane	110-82-7	16.87	16.30	17.30	0.05	56.1>41.1	9	84.1>41.1	18
3-Methylhexane	589-34-4	17.00	16.30	17.30	0.05	71.1>43.1	6	43.1>27.1	10
Carbon Tetrachloride	56-23-5	17.11	16.30	17.30	0.05	117.0>82.0	26	119.0>84.0	26
Benzene	71-43-2	17.58	17.30	17.93	0.1	78.1>52.0	18	77.1>51.0	18
2,2,4-Trimethylpentane	540-84-l	17.66	17.30	17.93	0.1	57.1>29.1	9	56.1>41.1	9
Ethylene dichloride (1,2-dichloroethane)	107-06-2	17.78	17.30	17.93	0.1	62.0>27.1	17	64.0>27.1	17
n-Heptane	142-82-5	18.13	17.93	18.73	0.15	43.1>27.1	6	71.1>43.1	10
Fluorobenzene (IS)	462-6-6	18.31	17.93	18.73	0.15	96.1>70.1	18		
Trichloroethylene	79-01-6	19.24	18.73	19.56	0.3	130.0>95.0	17	132.0>97.0	17
Methylcyclohexane	108-87-2	19.83	19.56	20.27	0.15	83.1>55.1	9	98.1>55.1	15
1,2-Dichloropropane	78-87-5	19.92	19.56	20.27	0.15	63.0>27.1	17	62.0>27.1	17
2,3,4-Trimethylpentane	565-75-3	20.64	20.27	20.85	0.3	71.1>43.1	7	43.1>27.1	10
2-Methylheptane	592-27-8	21.07	20.85	21.27	0.3	57.1>29.1	10	99.1>57.1	6
3-Methylheptane	589-81-1	21.43	21.27	21.89	0.15	85.1>43.1	7	57.1>29.1	9
cis-1,3-Dichloropropene	10061-01-5	21.57	21.27	21.89	0.15	110.0>75.0	8	75.0>49.1	17
Toluene-d8 (IS)	2037-26-5	22.21	21.89	22.71	0.1	98.1>70.2	16		
Toluene	108-88-3	22.39	21.89	22.71	0.1	92.1>91.1	6	91.1>65.1	16
n-Octane	111-65-9	22.50	21.89	22.71	0.1	85.1>43.1	8	43.1>27.1	10
trans-1,3-Dichloropropene	542-75-6	22.89	22.71	23.15	0.3	110.0>75.0	8	75.0>49.1	17
1,1,2-Trichloroethane	79-00-5	23.36	23.15	24.08	0.15	97.0>61.0	17	83.0>47.1	26
Tetrachloroethylene	127-18-4	23.56	23.15	24.08	0.15	166.0>131.0	17	164.0>129.0	17
Ethylene dibromide (1,2-dibromoethane)	106-93-4	24.50	24.08	24.90	0.3	107.0>27.1	18	109.0>27.1	18
Chlorobenzene-d5 (IS)	3114-55-4	25.23	24.90	25.96	0.06	117.1>82.1	18		0
Chlorobenzene	108-90-7	25.29	24.90	25.96	0.06	112.0>77.0	17	114.0>77.0	17

Compounds	CAS#	Rt (min)	MRM						
			Start time (min)	End (min)	Event (sec)	Target transition (*m/z*)	CE (V)	Qualifoer transition (*m/z*)	CE (V)
Ethylbenzene	100-41-4	25.40	24.90	25.96	0.06	106.1>91.1	10	91.1>65.1	18
n-Nonane	111-84-2	25.51	24.90	25.96	0.06	85.1>43.1	9	43.1>27.1	10
m-Xylene	108-38-3	25.61	24.90	25.96	0.06	106.1>91.1	15	91.1>65.1	18
p-Xylene	106-42-3	25.61	24.90	25.96	0.06	106.1>91.1	15	91.1>65.1	18
o-Xylene	95-47-6	26.25	25.96	26.58	0.15	106.1>91.1	15	91.1>65.1	18
Styrene	100-42-5	26.30	25.96	26.58	0.15	104.1>103.1	3	104.1>78.1	18
Isopropylbenzene (cumene)	98-82-8	26.81	26.58	27.09	0.3	105.1>77.1	18	120.1>105.1	9
1,1,2,2-Tetrachloroethane	79-34-5	27.25	27.09	27.83	0.043	168.0>83.0	8	166.0>83.0	8
α-Pinene	80-56-8	27.30	27.09	27.83	0.043	93.1>77.1	15	121.1>93.1	9
n-Propylbenzene	103-65-1	27.43	27.09	27.83	0.043	91.1>65.1	18	120.1>91.1	10
3-Ethyltoluene	620-14-4	27.53	27.09	27.83	0.043	105.1>77.1	18	120.10105.1	12
n-Decane	124-18-5	27.56	27.09	27.83	0.043	57.1>29.1	10	43.1>27.1	10
4-Ethyltoluene	622-96-8	27.61	27.09	27.83	0.043	105.1>77.1	18	120.1>105.1	12
1,3,5-Trimethylbenzene	108-67-8	27.67	27.09	27.83	0.043	120.1>105.1	15	105.1>77.1	18
2-Ethyltoluene	611-14-3	27.95	27.83	28.09	0.3	105.1>77.1	18	120.1>105.1	12
1,2,4-Trimethylbenzene	95-63-6	28.20	28.09	28.51	0.15	120.1>105.1	15	105.1>77.1	18
β-Pinene	127-91-3	28.38	28.09	28.51	0.15	121.1>106.1	15	93.1>77.0	12
m-Dichlorobenzene	541-73-1	28.67	28.51	29.05	0.06	146.0>111.1	17	148.0>113.1	17
1,2,3-Trimethylbenzene	526-73-8	28.76	28.51	29.05	0.06	120.1>105.1	15	105.1>77.1	18
p-Dichlorobenzene	106-46-7	28.82	28.51	29.05	0.06	146.0>111.1	17	148.0>113.1	17
Benzyl chloride	100-44-7	28.92	28.51	29.05	0.06	126.0>91.1	10	91.1>65.1	17
1,3-Diethylbenzene	141-93-5	28.96	28.51	29.05	0.06	105.1>77.1	18	119.1>91.1	12
1,4-Diethylbenzene	105-05-5	29.11	29.05	30.21	0.1	119.1>91.1	12	105.1>77.1	18
n-Undecane	1120-21-4	29.12	29.05	30.21	0.1	57.1>29.1	10	43.1>27.1	10
o-Dichlorobenzene	95-50-1	29.26	29.05	30.21	0.1	146.0>111.1	17	148.0>113.1	17
1,2,4-Trichlorobenzene	120-82-1	31.14	30.21	32.00	0.15	179.9>109.1	17	181.9>147.1	26
Hexachlorobutadiene	87-68-3	31.23	30.21	32.00	0.15	226.8>191.8	17	224.9>189.9	17

*1 Pseudo-MRM is a measurement method where ions with the same mass are selectively measured as precursor ions and product ions. Its advantage in principle is that allows the removal of contaminant ions in the collision cell.

Table 1-5 SIM, Product Ion Scan, MRM, Pseudo-MRM [*1] Methods

Compounds	CAS#	Rt (min)	Pseudo-MRM						
			Start (min)	End (min)	Event (sec)	Target transition (*m/z*)	CE (V)	Qualifier transition (*m/z*)	CE (V)
1.1.1.2-Tetrafluoroethane (HFC134a)	811-97-2	4.85	4.75	5.35	0.03	69.0>69.0	0	83.0>83.0	0
n-Propane	115-07-1	4.99	4.75	5.35	0.03	29.0>29.0	0	43.0>43.0	0
Propylene	74-98-6	5.00	4.75	5.35	0.03	41.1>41.1	0	39.0>39.0	0
Dichlorodifluoromethane (CFC12)	75-71-8	5.10	4.75	5.35	0.03	85.0>85.0	0	87.0>87.0	0
Chlorodifluoromethane (HCFC22)	75-45-6	5.14	4.75	5.35	0.03	51.0>51.0	0	67.0>67.0	0
Dichlorotetrafluoroethane (CFC114)	76-14-2	5.53	5.35	5.88	0.03	85.0>85.0	0	135.0>135.0	0
Isobutane	75-28-5	5.58	5.35	5.88	0.03	43.1>43.1	0	57.1>57.1	0
1-Chloro-1,1-difluoroethane (HCFC142b)	75-68-3	5.60	5.35	5.88	0.03	65.0>65.0	0	85.0>85.0	0
Methyl chloride (chloromethane)	74-87-3	5.71	5.35	5.88	0.03	50.0>50.0	0	52.0>52.0	0
1-Butene	106-98-9	6.03	5.88	7.00	0.03	56.1>56.1	0	41.1>41.1	0
n-Butane	106-97-8	6.08	5.88	7.00	0.03	43.1>43.1	0	58.1>58.1	0
Vinyl chloride (chloroethene)	75-01-4	6.09	5.88	7.00	0.03	62.0>62.0	0	64.0>64.0	0
1,3-Butadiene	106-99-0	6.24	5.88	7.00	0.03	54.1>54.1	0	39.1>39.1	0
trans-2-Butene	624-64-6	6.36	5.88	7.00	0.03	41.1>41.1	0	56.1>56.1	0
cis-2-Butene	590-18-1	6.66	5.88	7.00	0.03	41.1>41.1	0	56.1>56.1	0
Methyl bromide (bromomethane)	74-83-9	7.21	7.00	7.41	0.03	93.9>93.9	0	96.0>96.0	0
Ethyl chloride (chloroethane)	75-00-3	7.57	7.41	8.09	0.03	64.0>64.0	0	66.0>66.0	0
Isopentane (2-methylbutane)	78-78-4	7.79	7.41	8.09	0.03	43.1>43.1	0	42.1>42.1	0
Trichlorofluoroethane (CFC11)	75-69-4	8.34	8.09	8.84	0.03	101.0>101.0	0	102.9>102.9	0
1-Pentene	109-67-1	8.44	8.09	8.84	0.03	42.1>42.1	0	55.1>55.1	0
n-Pentane	109-66-0	8.61	8.09	8.84	0.03	43.1>43.1	0	42.1>42.1	0
trans-2-Pentene	646-04-8	9.06	8.84	9.71	0.03	55.1>55.1	0	70.1>70.1	0
1,1-Dichloro-1-fluoroethane (HCFC141b)	1717-00-6	9.22	8.84	9.71	0.03	81.0>81.0	0	83.0>83.0	0
2-Methyl-1,3-butadiene	78-79-5	9.38	8.84	9.71	0.03	67.0>67.0	0	53.0>53.0	0
cis-2-Pentene	627-20-3	9.39	8.84	9.71	0.03	55.1>55.1	0	70.0>70.0	0
2,2-Dichloro-1,1,1-trifluoroethane (HCFC123)	306-83-2	9.48	8.84	9.71	0.03	83.0>83.0	0	85.0>85.0	0
1,1,2-Trifluorotrichloroethane (CFC113)	76-13-1	9.95	9.71	10.38	0.03	101.0>101.0	0	151.0>151.0	0
Vinylidene chloride (1,1-dichloroethylene)	75-35-4	10.00	9.71	10.38	0.03	96.0>96.0	0	61.0>61.0	0
2,2-Dimethylbutane	75-83-2	10.09	9.71	10.38	0.03	43.1>43.1	0	57.1>57.1	0
3,3-Dichloro-1,1,1,2,2-pentafluoropropane (HCFC225ca)	422-56-0	10.74	10.38	10.99	0.03	83.0>83.0	0	85.0>85.0	0
Allyl chloride (3-chloro-1-propene)	107-05-1	11.18	10.99	11.99	0.03	41.1>41.1	0	39.1>39.1	0
1,3-Dichloro-1,1,2,2,3-pentafluoropropane (HCFC225cb)	507-55-1	11.35	10.99	11.99	0.03	67.0>67.0	0	69.0>69.0	0
2,3-Dimethylbutane	79-29-8	11.48	10.99	11.99	0.03	42.1>42.1	0	43.1>43.1	0
2-Methylpentane	107-83-5	11.54	10.99	11.99	0.03	43.1>43.1	0	42.1>42.1	0
Dichloromethane	75-09-2	11.56	10.99	11.99	0.03	49.0>49.0	0	84.0>84.0	0
Cyclopentane	287-92-3	11.76	10.99	11.99	0.03	42.1>42.1	0	55.1>55.1	0

Compounds	CAS#	Rt (min)	Pseudo-MRM						
			Start (min)	End (min)	Event (sec)	Target transition (*m/z*)	CE (V)	Qualifier transition (*m/z*)	CE (V)
Acrylonitrile	107-13-1	12.17	11.99	12.61	0.03	53.0>53.0	0	52.0>52.0	0
3-Methylpentane	96-14-0	12.34	11.99	12.61	0.03	57.1>57.1	0	56.1>56.1	0
2-Methyl-1-Pentene	763-29-1	12.84	12.61	14.17	0.03	56.1>56.1	0	41.1>41.1	0
n-Hexane	110-54-3	13.13	12.61	14.17	0.03	57.1>57.1	0	41.1>41.1	0
Ethylidene dichloride (1,1-dichloroethane)	75-34-3	13.73	12.61	14.17	0.03	63.0>63.0	0	65.0>65.0	0
2,4-Dimethyl-pentane	108-08-7	14.61	14.17	14.82	0.03	43.1>43.1	0	57.1>57.1	0
Methyl-cyclopentane	96-37-7	15.00	14.82	15.69	0.03	56.1>56.1	0	69.1>69.1	0
cis-1,2-Dichloroethene	156-59-2	15.25	14.82	15.69	0.03	61.0>61.0	0	96.0>96.0	0
Chloroform	67-66-3	16.15	15.69	16.35	0.03	83.0>83.0	0	85.0>85.0	0
2-Methylhexane	591-76-4	16.52	16.35	17.31	0.03	43.1>43.1	0	85.1>85.1	0
Methyl chloroform (1,1,1-trichloroethane)	71-55-6	16.65	16.35	17.31	0.03	97.0>97.0	0	99.0>99.0	0
2,3-Dimethylpentane	565-59-3	16.80	16.35	17.31	0.03	43.1>43.1	0	85.1>85.1	0
Cyclohexane	110-82-7	16.87	16.35	17.31	0.03	84.1>84.1	0	56.1>56.1	0
3-Methylhexane	589-34-4	17.00	16.35	17.31	0.03	43.1>43.1	0	71.1>71.1	0
Carbon Tetrachloride	56-23-5	17.11	16.35	17.31	0.03	116.9>116.9	0	118.9>118.9	0
Benzene	71-43-2	17.58	17.31	17.94	0.03	78.1>78.1	0	77.1>77.1	0
2,2,4-Trimethylpentane	540-84-l	17.66	17.31	17.94	0.03	57.1>57.1	0	56.1>56.1	0
Ethylene dichloride (1,2-dichloroethane)	107-06-2	17.78	17.31	17.94	0.03	62.0>62.0	0	64.0>64.0	0
n-Heptane	142-82-5	18.13	17.94	18.75	0.03	43.1>43.1	0	71.1>71.1	0
Fluorobenzene (IS)	462-6-6	18.31	17.94	18.75	0.03	96.1>96.1	0		
Trichloroethylene	79-01-6	19.24	18.75	19.52	0.03	129.9>129.9	0	131.9>131.9	0
Methylcyclohexane	108-87-2	19.83	19.52	20.29	0.03	83.1>83.1	0	55.1>55.1	0
1,2-Dichloropropane	78-87-5	19.92	19.52	20.29	0.03	63.0>63.0	0	62.0>62.0	0
2,3,4-Trimethylpentane	565-75-3	20.64	20.29	21.26	0.03	43.1>43.1	0	71.1>71.1	0
2-Methylheptane	592-27-8	21.07	20.29	21.26	0.03	57.1>57.1	0	43.1>43.1	0
3-Methylheptane	589-81-1	21.43	21.26	22.07	0.03	43.1>43.1	0	57.1>57.1	0
cis-1,3-Dichloropropene	10061-01-5	21.57	21.26	22.07	0.03	75.0>75.0	0	110.0>110.0	0
Toluene-d8 (IS)	2037-26-5	22.21	22.07	23.12	0.03	98.1>98.1	0		
Toluene	108-88-3	22.39	22.07	23.12	0.03	91.1>91.1	0	92.1>92.1	0
n-Octane	111-65-9	22.50	22.07	23.12	0.03	43.1>43.1	0	85.1>85.1	0
trans-1,3-Dichloropropene	542-75-6	22.89	22.07	23.12	0.03	110.0>110.0	0	75.0>75.0	0
1,1,2-Trichloroethane	79-00-5	23.36	23.12	24.08	0.03	97.0>97.0	0	83.0>83.0	0
Tetrachloroethylene	127-18-4	23.56	23.12	24.08	0.03	165.9>165.9	0	163.9>163.9	0
Ethylene dibromide (1,2-dibromoethane)	106-93-4	24.50	24.08	24.87	0.03	107.0>107.0	0	109.0>109.0	0
Chlorobenzene-d5 (IS)	3114-55-4	25.23	24.87	25.89	0.03	117.1>117.1	0		
Chlorobenzene	108-90-7	25.29	24.87	25.89	0.03	112.0>112.0	0	114.0>114.0	0
Ethylbenzene	100-41-4	25.40	24.87	25.89	0.03	91.1>91.1	0	106.1>106.1	0
n-Nonane	111-84-2	25.51	24.87	25.89	0.03	43.1>43.1	0	57.1>57.1	0
m-Xylene	108-38-3	25.61	24.87	25.89	0.03	91.1>91.1	0	106.1>106.1	0
p-Xylene	106-42-3	25.61	24.87	25.89	0.03	91.1>91.1	0	106.1>106.1	0
o-Xylene	95-47-6	26.25	25.89	27.05	0.03	91.1>91.1	0	106.1>106.1	0
Styrene	100-42-5	26.30	25.89	27.05	0.03	104.1>104.1	0	78.1>78.1	0
Isopropylbenzene (cumene)	98-82-8	26.81	25.89	27.05	0.03	105.1>105.1	0	120.1>120.1	0
1,1,2,2-Tetrachloroethane	79-34-5	27.25	27.05	27.81	0.03	83.0>83.0	0	85.0>85.0	0
α-Pinene	80-56-8	27.30	27.05	27.81	0.03	93.1>93.10	0	121.1>121.1	0
n-Propylbenzene	103-65-1	27.43	27.05	27.81	0.03	91.1>91.1	0	120.1>120.1	0
3-Ethyltoluene	620-14-4	27.53	27.05	27.81	0.03	105.1>105.1	0	120.1>120.1	0
n-Decane	124-18-5	27.56	27.05	27.81	0.03	57.1>57.1	0	43.1>43.1	0
4-Ethyltoluene	622-96-8	27.61	27.05	27.81	0.03	105.1>105.1	0	120.1>120.1	0
1,3,5-Trimethylbenzene	108-67-8	27.67	27.05	27.81	0.03	105.1>105.1	0	120.1>120.1	0
2-Ethyltoluene	611-14-3	27.95	27.81	28.06	0.03	105.1>105.1	0	120.1>120.1	0
1,2,4-Trimethylbenzene	95-63-6	28.20	28.06	28.48	0.03	105.1>105.1	0	120.1>120.1	0
β-Pinene	127-91-3	28.38	28.06	28.48	0.03	121.1>121.1	0	93.1>93.1	0
m-Dichlorobenzene	541-73-1	28.67	28.48	29.03	0.03	146.0>146.0	0	148.0>148.0	0
1,2,3-Trimethylbenzene	526-73-8	28.76	28.48	29.03	0.03	105.1>105.1	0	120.1>120.1	0
p-Dichlorobenzene	106-46-7	28.82	28.48	29.03	0.03	146.0>146.0	0	148.0>148.0	0
Benzyl chloride	100-44-7	28.92	28.48	29.03	0.03	126.0>126.0	0	91.0>91.0	0
1,3-Diethylbenzene	141-93-5	28.96	28.48	29.03	0.03	105.1>105.1	0	119.1>119.1	0
1,4-Diethylbenzene	105-05-5	29.11	29.03	30.28	0.03	119.1>119.1	0	105.1>105.1	0
n-Undecane	1120-21-4	29.12	29.03	30.28	0.03	57.1>57.1	0	43.1>43.1	0
o-Dichlorobenzene	95-50-1	29.26	29.03	30.28	0.03	146.0>146.0	0	148.0>148.0	0
1,2,4-Trichlorobenzene	120-82-1	31.14	30.28	32.00	0.03	179.9>179.9	0	181.9>181.9	0
Hexachlorobutadiene	87-68-3	31.23	30.28	32.00	0.03	224.9>224.9	0	226.8>226.8	0

*1 Pseudo-MRM is a measurement method where ions with the same mass are selectively measured as precursor ions and product ions. Its advantage in principle is that allows the removal of contaminant ions in the collision cell.

Table 2 Basis for Isomer Identification

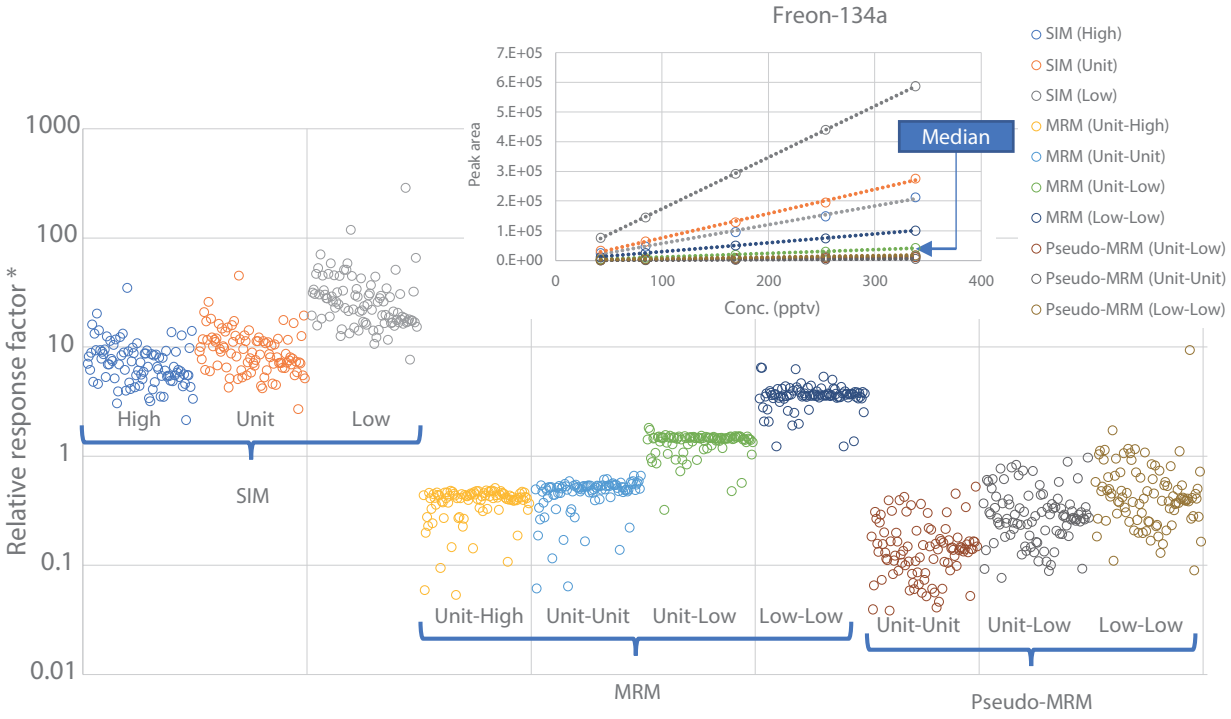
Elution Order	Compound Name	Molecular Formula	Basis for Identification
1	Isobutane	C4H10	Abundance ratio of ions *m/z* =27 and 29 similar to the NIST library data
2	1-Butene		
3	*n*-Butane	C4H8	Since there was no clear difference in the mass spectrum among the three isomers, the retention time obtained by measuring the standard gases prepared for two isomers individually
4	*trans*-2-Butene		
5	*cis*-2-Butene		
6	1-Pentene	C5H10	For 1-pentene and cyclopentane, the ion *m/z* =42, 55, and 70 profiles in particular are similar to NIST library data. Because distinct differences in the mass spectra of ***c***-2-pentene and ***t***-2-pentene and a degree of similarity to the NIST library data were not observed, the retention time obtained by measuring the standard gases prepared for each of them individually
7	*trans*-2-Pentene		
8	*cis*-2-Pentene		
9	Cyclopentane		
10	Isopentane	C5H12	Ion *m/z* = 43, 57, 72 profiles are similar to NIST library data
11	*n*-Pentane		
12	2-Methyl-1-pentene	C6H12	Ion *m/z* = 27, 29, 56, 69, 84 profiles are similar to NIST library data
13	Methylcyclopentane		
14	Cyclohexane		
15	2,2-Dimethylbutane	C6H14	Ion *m/z* = 41, 43, 55, 56, 71 profiles are similar to NIST library data
16	2,3-Dimethylbutane		
17	2-Methylpentane		
18	3-Methylpentane		
19	*n*-Hexane		
20	2,4-Dimethylpentane	C7H16	Ion *m/z* = 41, 42, 43, 56, 57, 70, 71, 72, 85 profiles are similar to NIST library data
21	2-Methylhexane		
22	2,3-Dimethylpentane		
23	3-Methylhexane		
24	*n*-Heptane		
25	2,2,4-Trimethyl pentane	C8H18	Ion *m/z* = 43, 57, 70, 71, 85, 91 profiles are similar to NIST library data
26	2,3,4-Trimethylpentane		
27	2-Methylheptane		
28	3-Methylheptane		
29	*n*-Octane		
30	Cumene (isopropylbenzene)	C9H12	Three among eight isomers - 4-ethyltoluene, 1,3,5-trimethylbenzene and 1,2,4-trimethylbenzene - were identified based on retention time because they were contained in the HAPs standard gas. For *n*-propylbenzene, isopropylbenzene and three isomers (3-ethyltoluene, 2-ethyltoluene and 1,2,3-trimethylbenzene), the ion *m/z* = 77, 91, 105 profiles are similar to the NIST library data. The remaining 3-ethyltoluene, 2-ethyltoluene, and 1,2,3-trimethylbenzene could not be determined from the mass spectrum, so were identified based on the retention time of the standard gases prepared for each of them individually.
31	*n*-Propylbenzene		
32	3-Ethyltoluene		
33	4-Ethyltoluene		
34	1,3,5-Trimethylbenzene		
35	2-Ethyltoluene		
36	1,2,4-Trimethylbenzene		
37	1,2,3-Trimethylbenzene		
38	1,3-Diethylbenzene	C10H14	Three isomers of xylene and three isomers of ethyl toluene are eluted in the order *m* -, *p* - so were identified according to this order of elution.
39	1,4-Diethylbenzene		
40	α-Pinene	C10H16	Abundance ratio of *m/z* =67 and 77 ions similar to NIST library data
41	β-Pinene		

3. Results

3-1. Differences in Detection Capability of Measurement Methods

Fig. 2 shows the results of comparing the sensitivity (ion current) of each method, taking as an index the slope of the absolute calibration curve generated by measuring standard gas (concentration of 42.6 pptv to 341 pptv, in 5 steps) in a method where the combination of MS measurement mode and mass resolution was changed. The relative response factor assigned to the vertical axis in the figure was standardized by dividing the slope obtained for each substance subject to measurement by its median. The ion currents were: SIM (Low) > SIM (Unit) > SIM (High) > MRM (Low-Low) > MRM (Unit-Unit) ≈ Pseudo > MRM (Low-Low) > MRM (Unit-High) ≈ Pseudo-MRM (Unit-Low) > Pseudo-MRM (Unit-Unit). With Pseudo-MRM (Unit-Unit), which was the least sensitive measurement mode, there was a failure to detect ethyl chloride at 42.7 pptv and acrylonitrile at 85.5 pptv. The detection capabilities of each method when they were compared by measuring environmental atmospheric samples and taking the total number of compounds that were under the lower limit of detection (peak vs. peak S/N < 3) as the index were: MRM (Low-Low) > MRM (Unit-Low) > SIM (Unit) > SIM (High) > MRM (Unit-Unit) > SIM (Low) > Pseudo-MRM (Unit-Low) > Pseudo-MRM (Low-Low) (Table 3).

The ranking order of the two results that pertained to detection capability did not match each other. This suggests that the MRM mode makes up for its low sensitivity (ion current) with its high selectivity.



* Relative response factor = Slope of absolute calibration curve /median slopes of 10 absolute calibration curve

Fig. 2 Sensitivity Comparison of Measurement Methods with Different Measurement Modes and Resolutions

Table 3 Number of Substances with S/N (Peak vs. Peak) of under 3 and Not Detectable, out of the 95 Substances Subject to Measurement

Measurement Mode	Optical Resolution	General Environment-1	General Environment-2	Roadside-1	Roadside-2	Vicinity of a Source-1	Vicinity of a Source-2	Total Substances Not Detectable
SIM	High	15	12	12	10	15	15	79
	Unit	9	10	10	10	13	15	67
	Low	16	14	14	13	17	10	84
MRM	Unit-Unit	15	11	13	11	16	17	83
	Unit-Low	9	8	8	9	9	11	54
	Low-Low	10	6	6	7	9	9	47
Pseudo-MRM	Unit-Low	23	19	24	18	25	26	135
	Low-Low	25	21	24	18	28	28	144

3-2. Differences in Selection Capability (Susceptibility to Ion Interference) Among Measurement Methods

As a result of measuring environmental atmospheric samples using methods with different measurement modes and resolutions, baseline drift, broad peaks and shoulder peaks, and changes in the ratio between quantifier ions (transition) and qualifier ions (transition) were observed in SIM chromatograms and MRM chromatograms of several substances subject to measurement due to differences in susceptibility to ion interference between contaminants and measured substances (Table 4). Of the substances subject to measurement that were not displayed, HCFC123, 1,1-dichloroethene, HCFC225cb, 1, 2-dibromoethane, and benzyl chloride were not detected in the environmental samples and it was not possible to evaluate differences in selectivity according to measurement method for them. No differences according to measurement method were observed for 26 substances including HFC134a and three internal standards. The measurement results using Pseudo-MRM were not evaluated because the S/N ratio of the component peaks to be measured was low compared to the SIM mode and MRM mode measurement results, and in addition to that no effect in reduction of ion interference compared to the SIM mode could be observed.

As you can see from the table, it was confirmed that setting the resolution to Unit-Unit in MRM mode measurement most effectively avoided the ion interference which was observed with other resolution settings and SIM mode measurement. On the other hand, there were substances that became undetectable upon setting to Unit-Unit, such as 2-methyl-1,3-butadiene. The inference from the results of this study is that accurate analysis can be achieved by making the resolution setting of the MRM method for VOC measurement Unit-Unit in principle, changing it to Unit-Low in cases where the concentration of the substance subject to measurement is low, and avoiding the Low-Low setting. However, for the transitions where baseline drift occurs when set to Unit-Low or Low-Low, i.e., 41 > 39, 75 > 49, 180 > 109, it is considered necessary to change the monitoring transition (Fig. 3).

Table 4 Issues with each Chromatogram that Hamper Qualitative/Quantitative Determinations

Substance Subject to Measurement for Which Issue Observed	Issue with Chromatogram that Hampers Qualitative/Quantitative Determination	SIM Mode	MRM Mode
		Resolution (Mass)	Resolution - Resolution (Transition)
n-Propane	Baseline drift	Low (43)	
Propylene	Peak non-detection		Unit-Unit and Unit-Low, Low-Low (29>15)
	Baseline drift		Low-Low (41>39)
HCFC22	Interference by Freon-12	Low (51)	Low (51>31, 57>31)
HCFC142b	Interference by an unknown substance (tailing peak)	Low (65)	
	Peak non-detection	Low (85)	
CFC114	Interference by isobutane	High, Unit, Low (85)	
Methyl chloride (chloromethane)	Interference by an unknown substance (tailing peak)	Low (50, 52)	
1-Butene	Interference by *n*-butane	High, Unit, Low (56, 41)	Unit-Unit, Unit-Low, Low-Low (56>41, 41>39)
	Baseline drift	Low (41)	Unit-Low, Low-Low (41>39)
Vinyl chloride (chloroethene)	Baseline drift	High, _Unit, _Low (64)	
trans-2-Butene	Baseline drift		Unit-Low, Low-Low (41>39)
cis-2-Butene	Interference by an unknown substance (shoulder peak)	Low (41)	
	Baseline drift		Unit-Low, Low-Low (41>39)
Methyl bromide (bromomethane)	Baseline drift	High, Unit, Low (96)	
Ethyl chloride (chloroethane)	Baseline drift	High, Unit, Low (66)	
Isopentane (2-methylbutane)	Baseline drift	Low (43, 42)	
	T/Q mismatch	High, Unit (43/42) and Low (43/42)	
1-Pentene	Baseline drift	Low (42)	
n-Pentane	Baseline drift	Low (43)	
	T/Q mismatch	High, Unit (43/42) and Low (43/42)	Unit-Unit, Unit-Low (43>27/42>27) and Low-Low (43>27/42>27)
trans-2-Pentene	Peak broadening, quantifier ion and qualifier ion retention time mismatch, interference by an unknown substance	Low (70)	
cis-2-Pentene	Mismatched T and Q retention time due to interference by an unknown substance	Low (70)	
2-Methyl-1,3-butadiene	Broad peak due to interference by an unknown substance	High, Unit, Low (67)	
	Peak non-detection		Unit-Unit (55>27)
2,2-Dimethylbutane	Interference by an unknown substance	High, Unit, Low (43)	Unit-Unit, Unit-Low, Low-Low (71>29)
HCFC225ca	Peak non-detection		Unit-Unit, Unit-Low, Low-Low (83>45, 85>49)
HCFC225cb	Interference by an unknown substance and 2,3-dimethylbutane, 2-methylpentane	Unit, Low (69)	
2,3-Dimethylbutane & 2-Methylpentane	Mutual interference	High, Unit, Low (42, 43)	Unit-Unit, Unit-Low, Low-Low (43>27, 43>15)
2-Methylpentane	Peak non-detection		Unit-Unit (71>41)

Substance Subject to Measurement for Which Issue Observed	Issue with Chromatogram that Hampers Qualitative/Quantitative Determination	SIM Mode	MRM Mode
		Resolution (Mass)	Resolution - Resolution (Transition)
Acrylonitrile	Interference by 3-methylpentane	High, Unit (53), Low (53, 52)	Unit-Low (53>26), Low-Low (53>26, 52>26)
2-Methyl-1-Pentene	Interference by an unknown substance	High, Unit, Low (41, 56)	Unit-Unit, Unit-Low, Low-Low (56>41)
Ethylidene dichloride	Baseline drift	High, Unit, Low (65)	
2,4-Dimethyl-pentane	Interference by an unknown substance	High, Unit, Low (43, 57)	Unit-Unit, Unit-Low, Low-Low (57>29)
cis-1,2-Dichloroethene	Interference by an unknown substance	High, Unit, Low (61)	
2-Methylhexane	Baseline drift	High, Unit, Low (43)	
Methyl chloroform	Interference by an unknown substance	High, Unit, Low (99)	
	Baseline drift	High, Unit, Low (97)	
2,3-Dimethylpentane	Interference by an unknown substance and cyclohexane	High, Unit, Low (56)	Low-Low (43>27)
Cyclohexane	Interference by an unknown substance (broad peak)	High, Unit, Low (56)	Unit-Unit, Unit-Low, Low-Low (56>41)
3-Methylhexane	Baseline drift	High, Unit, Low (43)	Unit-Unit, Unit-Low, Low-Low (43>27)
	Interference by an unknown substance and carbon tetrachloride	High, Unit, Low (43)	
Carbon Tetrachloride	T/Q mismatch	High and Unit (117/119), and Low (117/119)	
Benzene	T/Q mismatch	High and Unit (77/78) and Low (77/78)	Unit-Unit, Unit-Low (78>52/77>51), and Low-Low (78>52/77>51)
2,2,4-Trimethylpentane	Interference by an unknown substance	High, _Unit (56), _Low (56, 57)	Unit-Unit, Unit-Low, Low-Low (56>41)
n-Heptane	Baseline drift	High, Unit, Low (43)	
Trichloroethylene	Baseline drift	Low (132)	
Methylcyclohexane	Broad peak	SIM_Low (55)	
	T/Q mismatch	High and Unit (83/55) and Low (83/55)	
1,2-Dichloropropane	Interference by an unknown substance	Low (62)	
2,3,4-Trimethylpentane	Baseline drift	High, Unit, Low (43)	
2-Methylheptane	Interference by three types of unknown substance	High, Unit, Low (57, 43)	
	Interference by two types of unknown substance		Unit-Unit, Unit-Low, Low-Low (57>29)
	Interference by one type of unknown substance		Unit-Unit, Unit-Low, Low-Low (99>57)
	Baseline drift	High, _Unit, _Low (43)	Unit-Unit, Unit-Low, Low-Low (57>29)
3-Methylheptane	Baseline drift	High, Unit, Low (43)	
	Interference by an unknown substance		Unit-Low, Low-Low (85>43)
cis-1,3-Dichloropropene	Baseline drift	High, Unit, Low (75)	Low-Low (75>49)
trans-1,3-Dichloropropene	Interference by an unknown substance	Unit (75)	
	Peak non-detection	High, Unit, Low (110, 75)	
1,1,2-Trichloroethane	Interference by an unknown substance (shoulder peak)	High, Unit, Low (97, 83)	Unit-Unit, Unit-Low, Low-Low (83>47)
Chlorobenzene	Interference by chlorobenzene-d5	Low (114)	Low-Low (114>77)
Styrene	Interference by *o*-xylene	High, Unit, Low (104, 78)	Unit-Unit, Unit-Low, Low-Low (104>78)
	T/Q mismatch		Unit-Unit (104>103/104>78) and Unit-Low, Low-Low (104>103/104>78)
Isopropylbenzene	T/Q mismatch	High, Unit (105/120) and Low (105/120)	
n-Dacane	Interference by an unknown substance	High, Unit (43), Low (43, 57)	
β-Pinene	Interference by an unknown substance		Unit-Unit, Unit-Low, Low-Low (93>77)
m-Dichlorobenzene	Baseline drift	Low (146, 148)	
p-Dichlorobenzene	Baseline drift	Low (146, 148)	
1,3 -Diethylbenzene	Interference by an unknown substance	High, Unit, Low (105, 119)	Unit-Low, Low-Low (105>77, 119>91)
1,4-Diethylbenzene	Interference by an unknown substance	High, Unit (119), Low (105, 119)	Unit-Unit, Unit-Low, Low-Low (105>77, 119>91)
n-Undecane	Baseline drift	Low (43)	Unit-Unit, Unit-Low, Low-Low (57>29)
	Interference by an unknown substance	High, Unit, Low (57, 43)	Unit-Unit, Unit-Low, Low-Low (57>29)
o-Dichlorobenzene	Broad peak due to interference by an unknown substance	Low (146, 148)	
1,2,4-Trichlorobenzene	Peak non-detection	Low (180, 182)	
	Baseline drift		Low-Low (180>109)
Hexachlorobutadiene	Peak non-detection	High, _Unit, _Low (225, 227)	

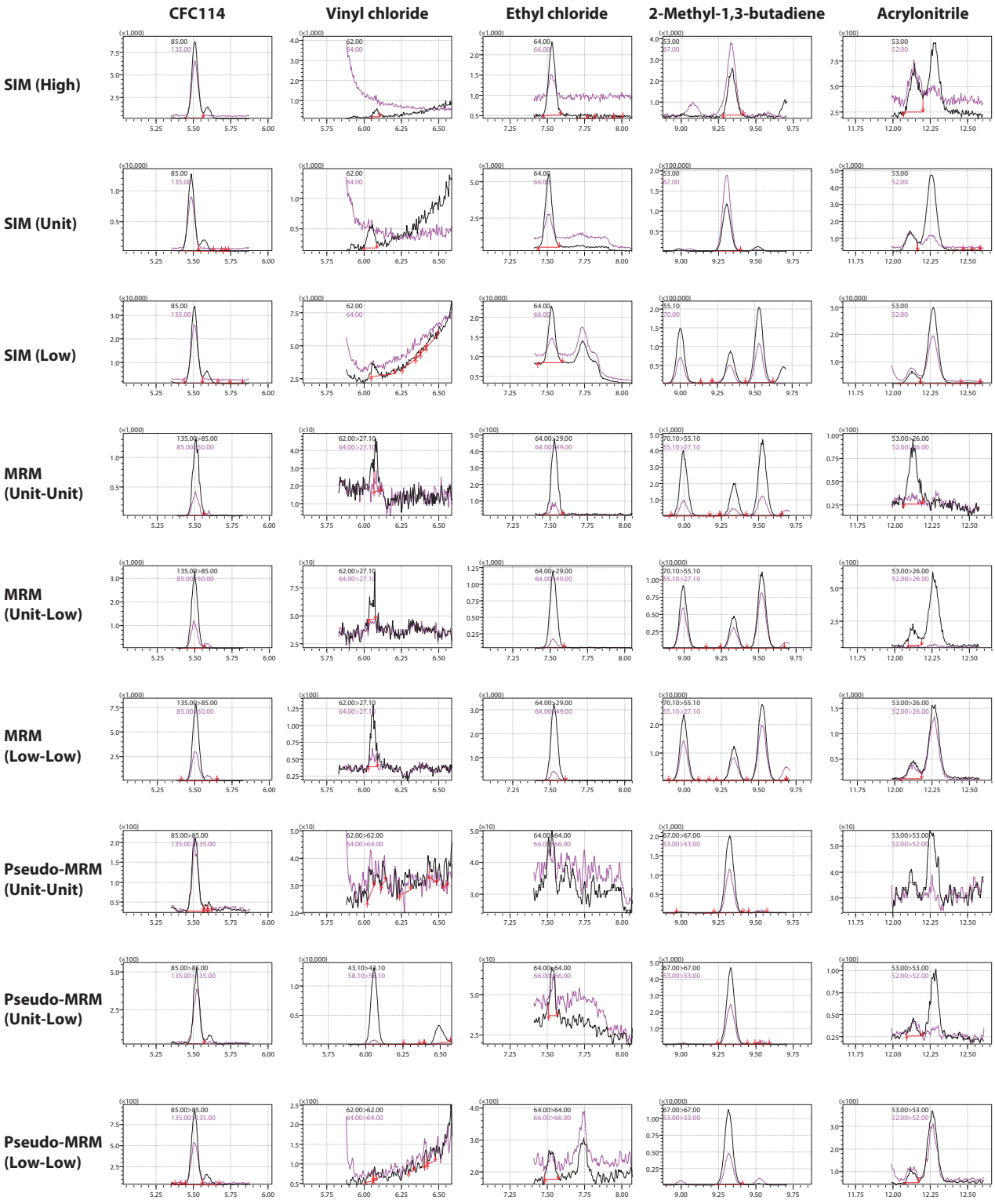


Fig. 3 Comparison of Chromatograms for Roadside Atmospheric Samples with Various Measurement Modes

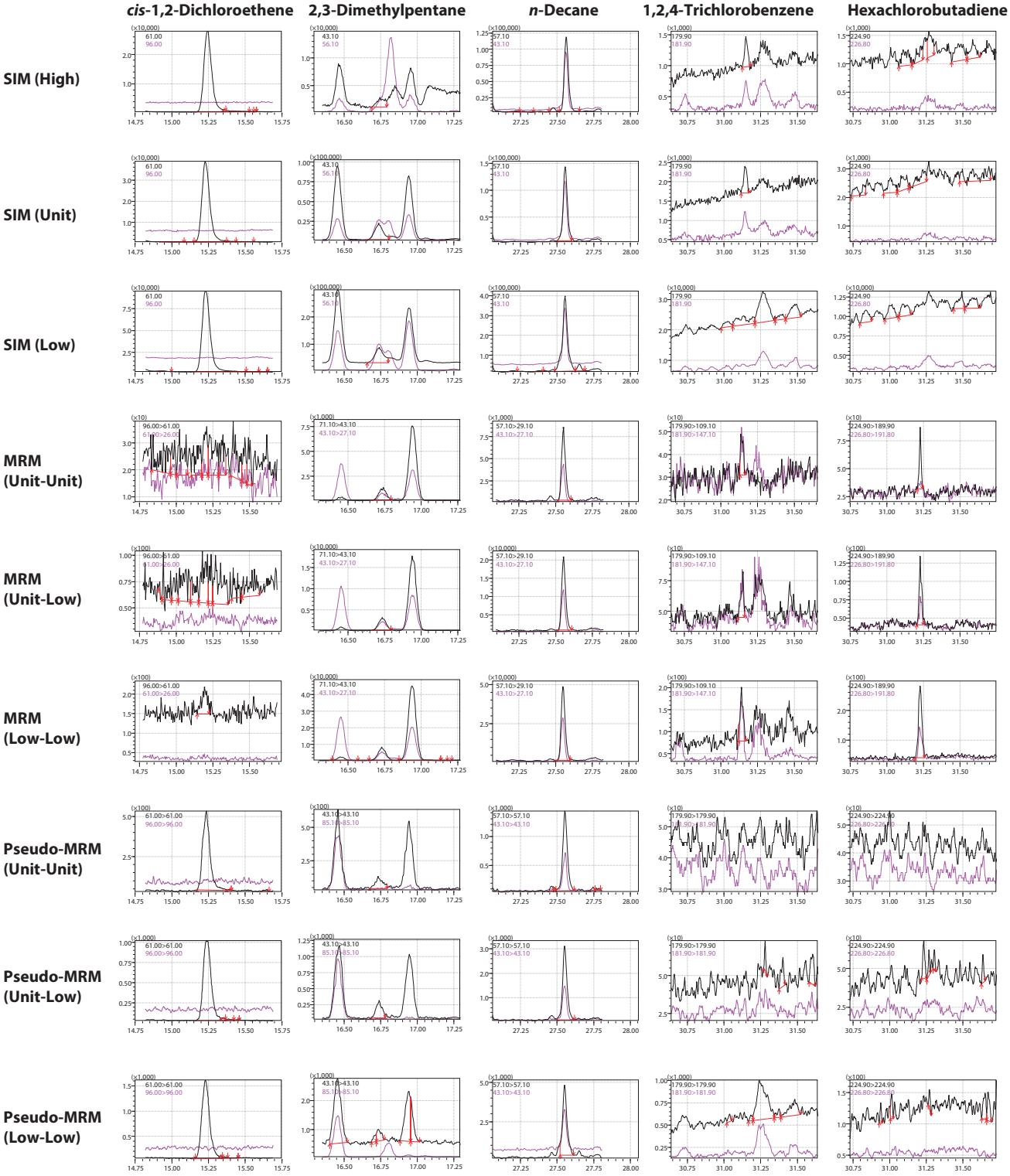


Fig. 3 Comparison of Chromatograms for Roadside Atmospheric Samples with Various Measurement Modes

4. Summary

In this study we were able to confirm that the GC/MS/MS method has superior detection capability to the SIM method, although it is inferior in terms of ion current. The remaining issues for future study include transition changes that may cause problems with qualitative and quantitative determinations listed in Table 4, adjustment of the EM voltage to improve sensitivity, and the appropriate smoothing method in the data processing of product ion scan chromatograms.

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