

# Analysis of 65 Volatile Organic Compounds in Ambient Air by Canister Sampling Using an Agilent 8890/5977 GC/MSD

A method using both scan and SIM mode that fully meets the requirements in the HJ 759-2023 standard

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## Abstract

This application note introduces the use of a canister for gas sampling. Samples were introduced into an Agilent 8890 gas chromatograph (GC) with an Agilent 5977 single quadrupole mass selective detector (MSD) and the Markes Multi-Gas thermal desorption (TD), to analyze volatile organic compounds (VOCs) in the atmosphere or in semiconductor cleanrooms. The results of linearity, reproducibility, and detection limit fully met the requirements of the China method HJ759-2023. This method is widely used as a reference both in environmental laboratories and semiconductor cleanrooms. The linear correlation coefficient for all 65 compounds was greater than 0.991, with 86% of compounds having a value greater than 0.999. The results of reproducibility in scan mode varied between 0.3 to 6.8%, while results in SIM mode varied between 1.1 to 6.7%. The sampling volume was 300 mL, which resulted in detection limits of 0.013 to 0.113 nmol/mol for scan mode and 0.002 to 0.013 nmol/mol for SIM mode.

## Introduction

VOCs are a common type of organic pollutant that are highly irritating and harmful, with a significant impact on the environment. The composition of VOCs in the atmospheric environment is complex and they are crucial contributors to the formation of photochemical smog in the air. The study of VOCs has become a focus both domestically and internationally, with many countries issuing a series of regulations for the monitoring of air quality. In China, Europe, America, and other places, the detection of VOCs in the environment is not only a key project for city, regional, or national environmental monitoring stations, but also for certain manufacturing enterprises. These manufacturers, such as wafer factories, require strict control of VOCs in cleanrooms. Currently, with the rapid development of semiconductor technology and chip production entering the nanometer scale, the corresponding requirements for the production environment are becoming successively greater. The control of molecular-level air pollutants in cleanroom environments is becoming increasingly urgent, and VOCs are one of the molecular-level air pollutants that need to be strictly controlled. The main sources of VOCs in cleanrooms include interior decoration materials, equipment materials, cleaning agents, outdoor air, etc.<sup>1</sup> VOC pollutants in the ambient air can cause contamination on the surface of semiconductor wafers, corrosion of connecting wires, and other problems that endanger product quality. Therefore, VOC pollutants have become a major factor affecting industrial development of wafers and their yield rate.

In the analysis of VOCs in ambient air, thermal desorption gas chromatography/mass spectrometry (TD-GC/MSD) is mostly used for detection both in environmental monitoring labs and semiconductor industry cleanrooms. There are two common ways to collect samples. One type of sampling involves the use of an adsorption tube for sample collection and preconcentration, followed by analysis through a TD-GC/MSD system. The HJ 734-2014<sup>2</sup> method specifies the use of adsorption tubes and TD-GC/MSD to detect 24 VOCs. Markes International has published an application note based on the HJ734 method, which shows excellent performance results using adsorption tube sampling method.<sup>3</sup> An alternative method employs a pre-evacuated canister for sample collection, with low-temperature condensation used for preconcentration. The HJ759-2023<sup>4</sup> standard provides a detailed description of a method using a canister for sampling and determining 65 VOCs in ambient air.

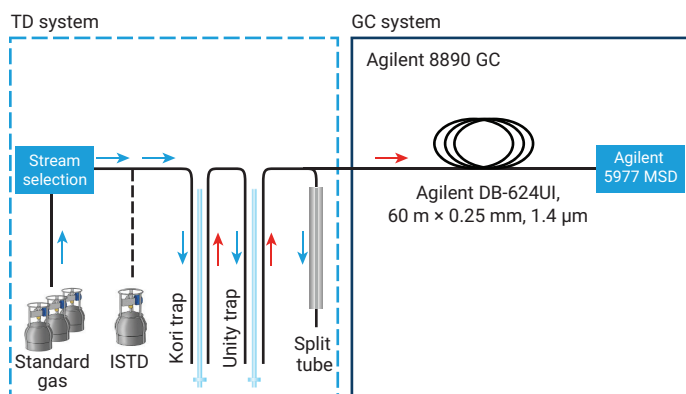
This study adopts the HJ759-2023 method as a reference, using canister sampling for the qualitative and quantitative analysis of 65 VOCs. Excellent linearity, high precision, and excellent reproducibility results were demonstrated, which shows the inertness of the full flow path, high sensitivity, and durability of the whole TD-GC/MSD system.

## Experimental

This study was performed on an 8890 GC coupled to a 5977 single quadrupole GC/MSD with an electron ionization (EI) source. A Markes Multi-Gas thermal desorption sample introduction and preconcentration system was used and included three modules:

- CIA Advantage-xr (CIA): canister autosampler
- Kori-xr: water removal module
- Unity-xr: thermal desorption instrument

First, three internal standards (ISTDs) were introduced into the Unity trap by CIA. Then, the sample was passed through a heated transfer line through the CIA Advantage into the Kori for water removal. Finally, the sample flowed into the focusing cold trap of the Unity for preconcentration. Eventually, the Unity trap was desorbed at high temperature, and the 65 VOCs and three ISTDs all entered the GC/MSD for analysis. Figure 1 shows the flow path of the combined system. Tables 1 and 2 illustrate the instrument conditions and consumables used in the system.



**Figure 1.** Schematic illustration of the flow path of a Markes TD and an Agilent 8890/5977 GC/MSD system.

**Table 1.** TD parameters.

Parameter	Value
Instrument	Multi-Gas UNITY-xr, Multi-Gas CIA Advantage xr, Kori-xr
Cold Trap	Markes HJ 759 (p/n U-HJ759-KXR)
<b>General</b>	
Flow Path Temperature	120 °C
Sampling Line Temperature	120 °C
<b>Presampling</b>	
Sample Purge Time	0.1 min
Sample Purge Flow	50 mL/min
Internal Standard Volume	30 mL
<b>Sampling</b>	
Sample Volume	30 to 300 mL
Sampling Flow	20, 50 mL/min
<b>Post Sampling Purge</b>	
Post Sampling Purge Time	4 min
Post Sampling Purge Flow	50 mL/min
CIA Post Sampling Purge Flow	50 mL/min
<b>Kori Settings</b>	
Kori Trap Low	-30 °C
Kori Trap High	300 °C
<b>Trap Settings</b>	
Trap Purge Time	1 min
Elevated Trap Purge Temperature	10 °C
Trap Purge Flow	50 mL/min
Trap Low Temperature	-25 °C
Trap High Temperature	250 °C
Trap Desorption Time	3 min
Desorb Split Flow	2 mL/min

**Table 2.** GC conditions.

Parameter	Value
<b>Agilent 8890 GC</b>	
Column	Agilent DB-624 UI, 60 m × 0.25 mm, 1.4 µm (p/n 122-1364 UI)
Carrier Gas	Helium, constant flow, 1 mL/min
Oven Program	35 °C (5 min), 5 °C/min to 150 °C (7 min), 10 °C/min to 200 °C (4 min)
<b>Agilent 5977 MSD</b>	
Ion Source Temperature	230 °C
Quad Temperature	150 °C
Tune File	Atune.u
Acquisition Type	Scan/SIM, m/z scan range 35 to 500
Gain Factor	1
Drawout Plate	6 mm

In this study, gas standards were purchased from Zhongce Standards Technology Co., Ltd. (Chengdu, China). One cylinder contained a mixed standard of 65 VOCs, each with a concentration approximating 1 µmol/mol. The other cylinder contained four compounds, three of which were ISTDs (bromochloromethane: ISTD 1; 1,4-difluorobenzene: ISTD 2; and chlorobenzene-d<sub>5</sub>: ISTD 3); the fourth compound was 4-bromofluorobenzene (BFB). All had concentrations of approximately 1 µmol/mol. BFB was required for injection during the tuning evaluation to learn if the entire system, particularly the mass spectrometer, was operating at optimal conditions. These two standard gas cylinders both used nitrogen as the balance gas.

### Preparation of 65 VOCs standard gas

Before establishing the calibration curve, the 1 µmol/mol standard gas had to be diluted to 0.5, 5, and 20 nmol/mol, respectively, and stored in canisters. According to the requirements of the HJ 759 method, to simulate real samples as much as possible, the standard gas also needed to be humidified. The relative humidity of the standard gas in canisters after final dilution was 50%. Therefore, after cleaning canisters, a certain amount of deionized water was added to the canisters according to the humidification method in Appendix B of HJ 759. Then, through a static dilution system using high-purity nitrogen (99.999% purity) as the dilution gas, the 1 µmol/mol standard gas was diluted to the target concentration levels. As shown in Tables 3 and 4, in scan mode, the target concentrations were 5 and 20 nmol/mol, respectively. In SIM mode, the target concentrations were 0.5 and 5 nmol/mol, respectively. Then different volumes were pumped in by the CIA to obtain calibration levels with different concentrations.

**Table 3.** Preparation of calibration mixture of 65 VOCs for scan mode.

Scan	5 nmol/mol			20 nmol/mol		
Sample Volume (mL)	30	60	150	60	150	300
Calibration Levels (nmol/mol)	0.5	1	2.5	4	10	20

**Table 4.** Preparation of calibration mixture of 65 VOCs for SIM mode.

SIM	0.5 nmol/mol			5 nmol/mol		
Sample Volume (mL)	60	150	300	60	150	300
Calibration Levels (nmol/mol)	0.1	0.25	0.5	1	2.5	5

## Preparation of ISTD gas

The 1  $\mu\text{mol/mol}$  ISTD was directly diluted to 50 nmol/mol with high purity nitrogen. The sample volume pumped into the system was 300 mL, as detailed in the HJ 759 method. By pumping 30 mL into the system through the CIA, the corresponding concentration of the internal standards distributed in a 300 mL sample was 5 nmol/mol.

The HJ 759 method requires the use of canisters for sample collection. Some of the 65 VOCs have high polarity and were easily adsorbed; it was therefore necessary to use passivated canisters. Moreover, the canisters had to rigorously be cleaned before use to reduce their own adsorption of polar or high-boiling point compounds. It is suggested to prepare a canister filled with high purity nitrogen. Before each batch of samples is run, a blank check of the canister and the system should be carried out.

## Results and discussion

### TD parameter optimization

To simulate the humidity of real samples, the standard gas was also subjected to 50% humidification treatment during preparation. The UNITY-CIA Advantage-xr Kori-xr instrument employs Dry Focus3 for effective management of humidity from gas phase samples, ensuring robust results, extending the life of the GC column and prolonging source cleaning of the MSD.

Dry Focus3 is a fully automated three-stage process for drying, focusing, and injecting humid samples. Figure 2 shows the three-stage process. Step 2 takes advantage of a temperature-programmed purge of the cold trap to eliminate residual water retained by the strong sorbents required for HJ 759. Even small amounts of residual water can affect the

### Step 1 – Sampling

The sample passes through a drying trap to selectively remove water before concentration of the analytes on the focusing trap.

### Step 2 – Trap purge

A temperature-programmed purge of the focusing trap allows elimination of residual water while retaining all trapped analytes.

### Step 3 – Desorption

The focusing trap heats rapidly in a reversed flow of carrier gas to inject analytes into the GC column. At the same time, the drying trap is regenerated for the next sample.

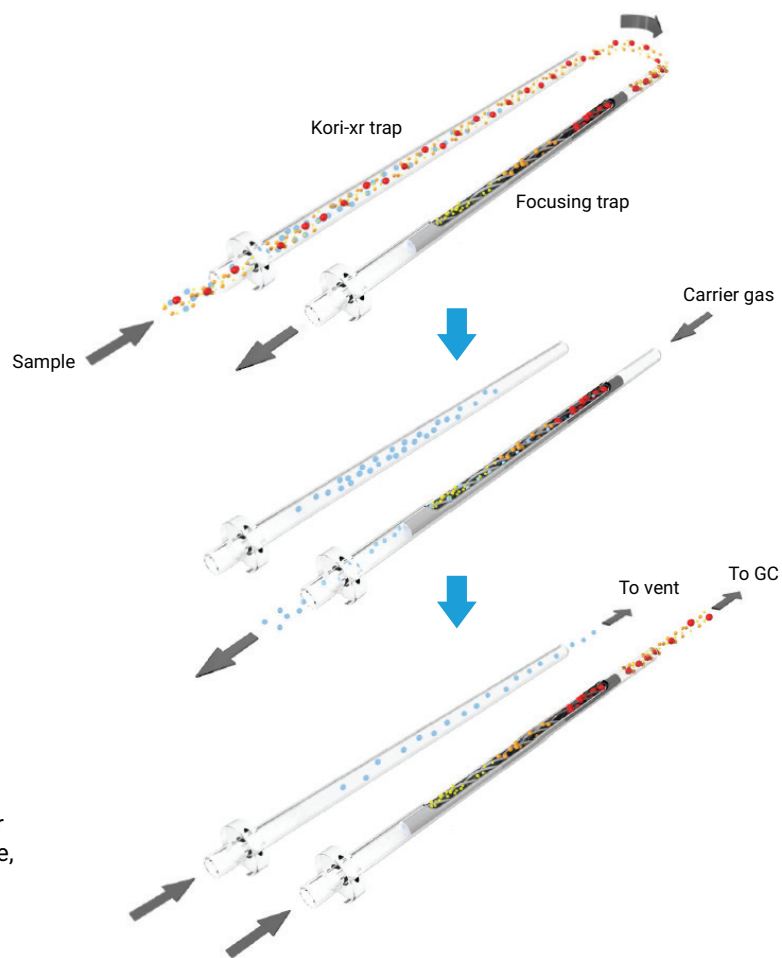
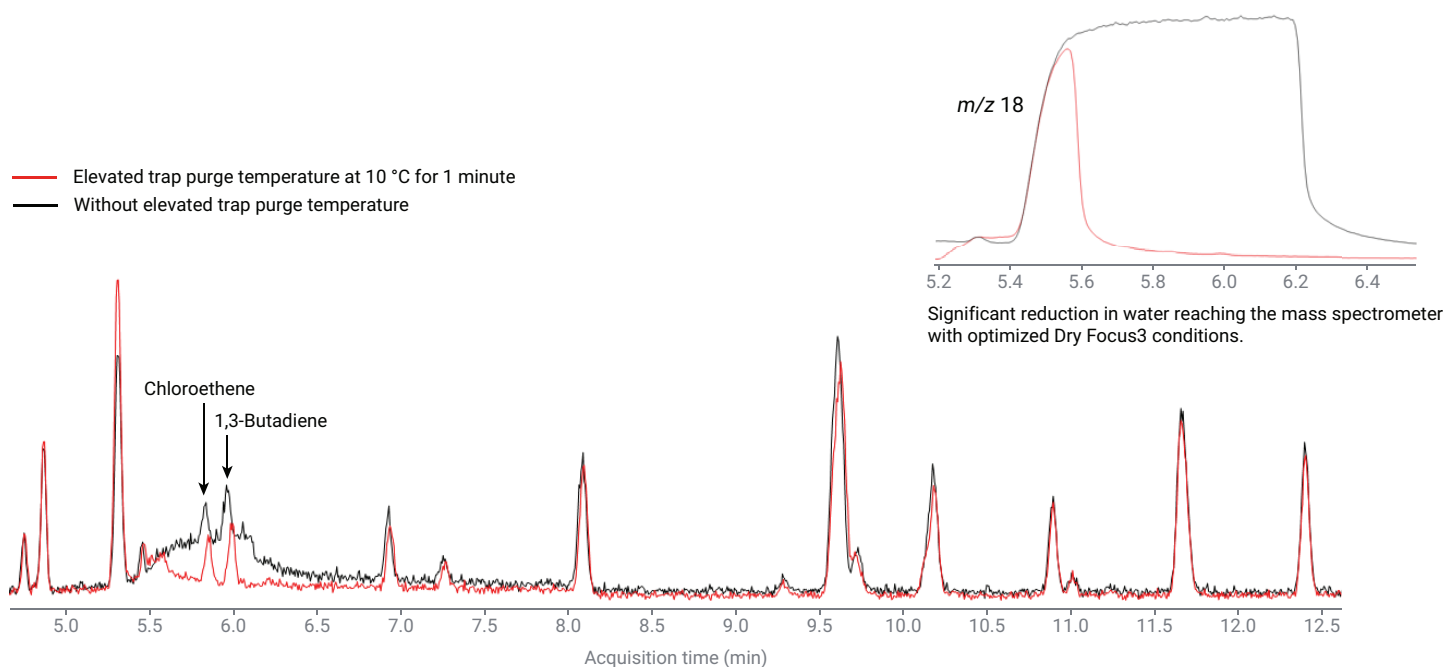


Figure 2. The schematic shows the whole process of Dry Focus3.

ionization efficiency of the mass spectrometer, impacting target compounds that coelute with water to the greatest degree. In this study, analyte trapping at  $-25\text{ }^{\circ}\text{C}$  ensured sensitive detection of target compounds while an elevated temperature purge was optimized to eliminate residual water. The higher the purge temperature and the longer the time, the sooner the more volatile targets will begin to breakthrough

to be lost from the Unity trap. If the purge temperature is too low or the time is too short, effective water removal is not achieved. Optimized elevated temperature purge conditions of  $10\text{ }^{\circ}\text{C}$  and  $50\text{ mL/min}$  purge flow for 1 minute are shown in Figures 3 and 4; this balances retention of the most volatile target analytes with efficient water removal.



**Figure 3.** Comparison of chromatograms in scan mode (scan from  $m/z$  35) with and without "enable elevated trap purge temperature" function. For the water check, scan from  $m/z$  12.



**Figure 4.** Enable the "elevated trap purge temperature" function in TD software.

## Scan mode results

Scan mode is used for combined qualitative analysis of unknown compounds along with targeted quantitative analysis. With the library search function, the mass spectrum of the unknown peak can be compared with the standard mass spectrum in the library, providing preliminary qualitative results. Figure 5 is the total ion chromatogram (TIC) of 2.5 nmol/mol standard gas obtained under the full scan mode for 65 VOCs. All compound peaks are sharp and symmetrical. For some polar compounds, such as 1,4-dioxane and isopropanol, the peak shape remains outstanding even when the relative humidity of the sample is 50%. Most compounds have achieved baseline separation, while a small number of the compounds are coeluted. Because different quantitative ions can be selected during quantification, it does not affect accurate qualitative and quantitative analysis. In Figure 5, in addition to the 65 VOCs and three ISTDs, there is also a BFB peak. This is because BFB was prepared with three internal standard substances in a standard gas cylinder, so the peak of BFB can be seen in scan mode. In contrast, in SIM mode, only the ions of the target substance and the ISTD substance were collected, so the BFB peak could not be found in the TIC in SIM mode (Figure 7).

The calibration curves were developed based on the ISTD method for six concentration levels from 0.5 to 20 nmol/mol. The 6 mm drawout plate was used for the best linearity for all compounds. For each component at every level of calibration, an average relative response factor (RRF) was determined with the ISTD method. The RRF for the percent relative standard deviation (%RSD) was less than 28% for all substances analyzed. In relation to linear curve fitting, the correlation coefficient ( $R^2$ ) was found to be at least 0.994 for each component, as shown in Table 5.

Repeatability was assessed by calculating the relative standard deviation (RSD) of the area from eight replicate runs at 0.5 nmol/mol (low), 2.5 nmol/mol (middle), and 10 nmol/mol (high) concentration levels (Figure 6). Table 5 shows the overall area %RSD was 0.3 to 6.8 %. For middle and high concentration levels, the area %RSD of most compounds was less than 3%. For low concentration, due to the smaller peak area, the RSD would be slightly larger, with the %RSD of most compounds ranging between 3 to 4%.

In this study, the method detection limit (MDL) was established by conducting eight replicated tests using a 0.5 nmol/mol standard gas. The concentration of each compound was calculated using a linear equation, followed by the calculation of the standard deviation and multiplication by 3 to determine the MDL. The study showed that the calculated detection limits for 65 VOCs ranged from 0.013 to 0.113 nmol/mol, as shown in Table 5.

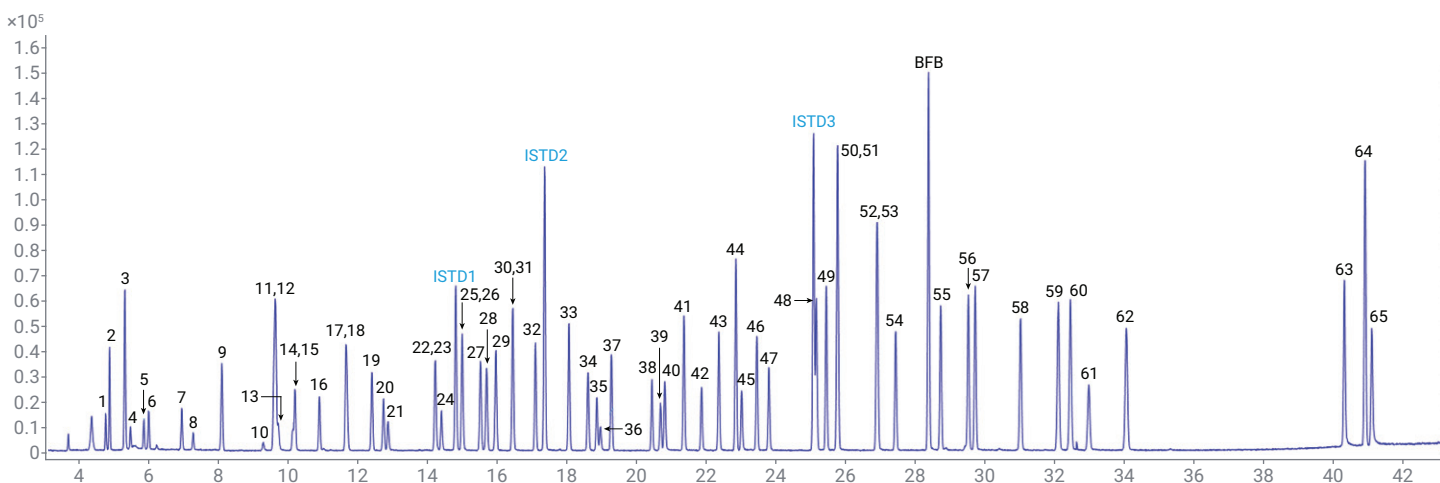


Figure 5. Total ion chromatogram of 65 VOCs at the concentration of 2.5 nmol/mol in scan mode

**Table 5.** Linearity, repeatability, and MDL results for 65 VOCs in scan mode (continued on the next page).

No.	Name	RT	m/z	RRF %RSD	CF R2	Area %RSD			MDL (nmol/mol)	ISTD
						Low	Mid	High		
1	Propene	4.813	41	5.7	0.9984	1.9	1.5	1	0.039	1
2	Dichlorodifluoromethane	4.929	85	3.1	0.9996	2.9	0.9	1	0.032	1
3	1,1,2,2-Tetrafluoro-1,2-dichloroethane	5.36	134.9	3.3	0.9993	2.7	1.2	1	0.041	1
4	Chloromethane	5.515	50	8.1	0.9956	6.3	2.5	1	0.113	1
5	Chloroethene	5.921	62	3.4	0.9996	2.7	0.8	1	0.040	1
6	1,3-Butadiene	6.045	54	4.3	0.9997	5.1	1.9	1	0.072	1
7	Bromomethane	7.00	94	7.2	0.9941	5.1	0.8	1	0.069	1
8	Chloroethane	7.331	64	3.6	0.9997	4.4	1.7	1	0.056	1
9	Trichlorofluoromethane	8.134	101	3.6	0.9995	2.3	0.3	1	0.039	1
10	Acrolein	9.325	56.1	8.6	0.9997	6.6	2	1	0.067	1
11	1,1-Dichloroethylene	9.63	96	5.0	0.9997	3.6	1.4	1	0.050	1
12	1,2,2-Trifluoro-1,1,2-trichloroethane	9.671	150.9	2.8	0.9995	2.9	1.3	1	0.047	1
13	Acetone	9.762	58	2.2	0.9999	4.1	1.5	1	0.064	1
14	Isopropyl alcohol	10.187	45	7.5	0.9988	4.6	1.3	1	0.056	1
15	Carbon disulfide	10.236	76	3.1	0.9997	2	0.8	1	0.023	1
16	Dichloromethane	10.937	84	3.8	0.9996	3.4	1.6	1	0.041	1
17	<i>trans</i> -1,2-Dichloroethylene	11.693	96	4.3	0.9996	5.1	1.6	1	0.072	1
18	Methyl tert-butyl ether	11.73	73	9.0	0.9997	3.1	1.6	1	0.033	1
19	<i>n</i> -Hexane	12.435	57	6.1	0.9997	2.8	1.4	1	0.033	1
20	1,1-Dichloroethane	12.766	63	3.9	0.9995	2	1.4	1	0.039	1
21	Vinyl acetate	12.9	43	13.2	0.9996	4.3	1.3	1	0.044	1
22	<i>cis</i> -1,2-Dichloroethylene	14.246	96	4.1	0.9997	2	1.3	1	0.027	1
23	2-Butanone	14.272	72	8.6	0.9997	6.8	1.3	1	0.068	1
24	Ethyl Acetate	14.433	43	10.1	0.9998	5.3	2	1	0.059	1
25	Trichloromethane	15.02	83	4.5	0.9998	1.7	0.7	2	0.041	2
26	Tetrahydrofuran	15.038	72	12.3	0.9997	5.8	1.3	1	0.058	1
27	1,1,1-Trichloroethane	15.548	97	3.1	0.9998	3.3	0.7	2	0.048	2
28	Cyclohexane	15.721	84	5.9	0.9997	2.8	1.9	2	0.027	2
29	Carbon Tetrachloride	15.983	116.9	3.3	0.9997	3	1.1	2	0.031	2
30	1,2-Dichloroethane	16.471	62	4.4	0.9999	3.1	1.2	2	0.048	2
31	Benzene	16.471	78	5.3	0.9998	1.2	0.5	2	0.031	2
32	Heptane	17.117	43	6.8	0.9998	4.1	1.4	2	0.046	2
33	Trichloroethylene	18.081	130	5.9	0.9999	2.9	1.1	2	0.042	2
34	1,2-Dichloropropane	18.627	63	2.7	0.9999	3.3	1.7	2	0.039	2
35	Methyl methacrylate	18.888	100.1	17.4	0.9991	4.8	1.7	2	0.058	2
36	1,4-Dioxane	18.995	88	11.3	0.9951	3.5	2.3	2	0.058	2
37	Bromodichloromethane	19.296	83	4.0	0.9999	3.1	1.1	2	0.041	2
38	<i>cis</i> -1,3-Dichloropropene	20.459	75	6.7	0.9996	3	0.7	2	0.045	2
39	Dimethyl disulfide	20.709	94	17.2	0.9978	3.8	2.1	2	0.027	2
40	Methyl isobutyl ketone	20.839	43	8.6	0.9991	3.2	1.7	2	0.040	2
41	Toluene	21.376	91	4.4	0.9999	1.4	1.1	2	0.027	2
42	<i>trans</i> -1,3-Dichloropropene	21.882	75	8.5	0.9997	2.9	1.2	2	0.036	2
43	1,1,2-Trichloroethane	22.38	96.9	3.2	0.9997	1.7	1.1	2	0.032	2
44	Tetrachloroethylene	22.863	165.8	5.6	0.9997	1.6	0.8	2	0.046	2
45	2-Hexanone	23.042	43	12.4	0.9989	3.7	1.2	2	0.047	2

No.	Name	RT	m/z	RRF %RSD	CF R2	Area %RSD			MDL (nmol/mol)	ISTD
						Low	Mid	High		
46	Dibromochloromethane	23.467	128.8	4.5	0.9998	1.7	1	2	0.029	2
47	1,2-Dibromoethane	23.815	106.9	3.9	0.9999	2.6	1.8	2	0.041	2
48	Chlorobenzene	25.169	112	3.2	0.9999	1.4	1.2	3	0.019	3
49	Ethylbenzene	25.455	91	6.9	0.9998	2.5	0.8	3	0.020	3
50,51	<i>m,p</i> -Xylene	25.778	91	8.9	0.9998	2.4	0.8	3	0.013	3
52	<i>o</i> -Xylene	26.898	91.1	9.3	0.9998	3.1	0.8	3	0.027	3
53	Styrene	26.924	104	15.3	0.9997	3.4	0.4	3	0.027	3
54	Bromoform	27.449	173	6.2	0.9997	3.2	1.3	3	0.036	3
55	1,1,2,2-Tetrachloroethane	28.735	83	6.4	0.9997	3.3	1.1	3	0.034	3
56	<i>p</i> -Ethyltoluene	29.528	105.1	17.6	0.9996	1.8	1.7	3	0.016	3
57	1,3,5-Trimethylbenzene	29.729	105.1	19.6	0.9997	3.1	1.7	3	0.024	3
58	1,2,4-Trimethylbenzene	31.029	105	22.3	0.9996	4.7	1.3	3	0.029	3
59	1,3-Dichlorobenzene	32.115	146	8.4	0.9998	3.4	1	3	0.032	3
60	1,4-Dichlorobenzene	32.46	146	9.3	0.9998	3.8	0.9	3	0.032	3
61	Benzyl chloride	32.984	91	27.8	0.9988	3.2	1.4	3	0.024	3
62	1,2-Dichlorobenzene	34.065	145.9	10.3	0.9997	3.6	0.6	3	0.036	3
63	1,2,4-Trichlorobenzene	40.312	179.9	11.4	0.9992	4.7	2.6	3	0.054	3
64	Hexachlorobutadiene	40.908	224.8	11.3	0.9996	4.6	1.4	3	0.046	3
65	Naphthalene	41.101	128	22.4	0.9986	4.9	2.4	3	0.042	3

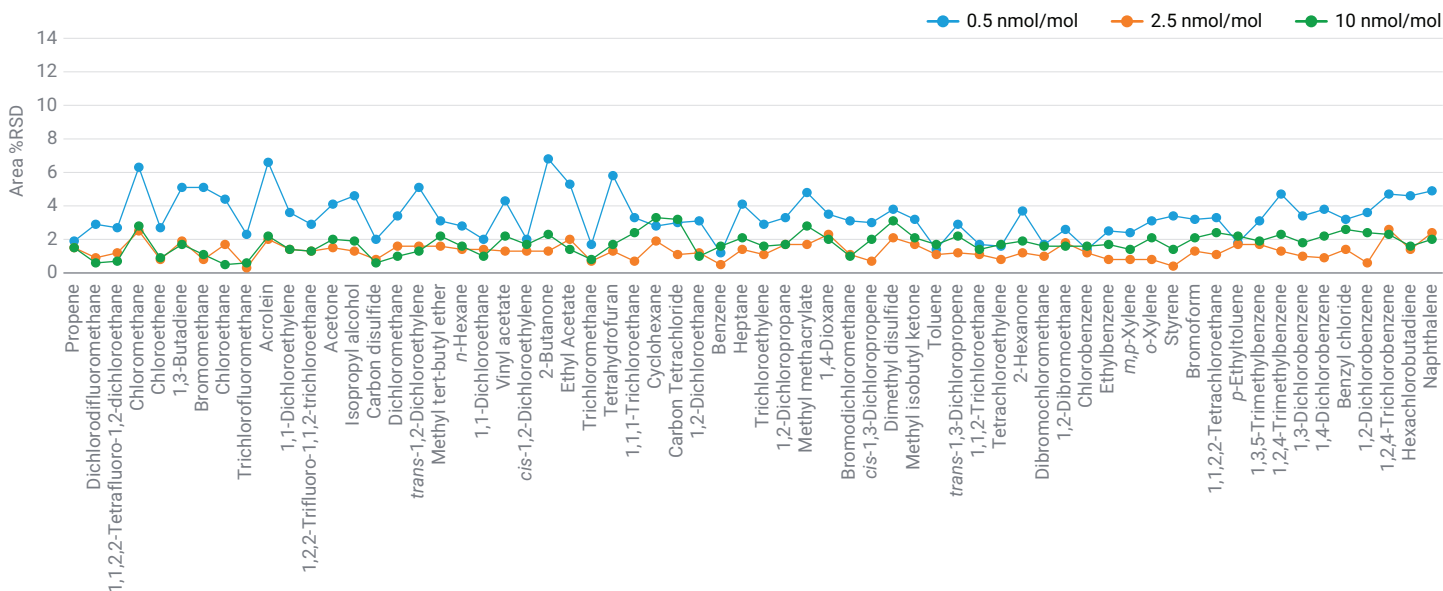


Figure 6. Repeatability results for 65 VOCs at low, middle, and high calibration levels in scan mode.



## SIM mode results

SIM mode uses a defined compound list to perform sensitive, targeted analysis. In SIM mode, it is necessary to group the target substances in advance and input the characteristic ions of each target substance to establish an acquisition method. Figure 7 is the TIC of the 1 nmol/mol standard gas collected under SIM mode. Because only the ions of interest are collected, only the chromatographic peaks of the target substances appear on the chromatogram. Therefore, compared to scan mode, the data collected in SIM mode have fewer interference peaks, and the BFB peak cannot be seen. Similar to scan mode data, under SIM mode, all compound peaks are also sharp and symmetrical, demonstrating the excellent inertness of the entire TD/GC/MSD system and fast injection from TD to GC.

In SIM mode, a comprehensive method evaluation was also performed. The linear range of SIM mode is from 0.1 to 5 nmol/mol, which is approximately 5x lower than the concentrations in scan mode. Within this linear range, the RRF %RSD was less than 22% for all substances analyzed. The correlation coefficient values of 84% of the compounds were greater than 0.999, while the remaining 16% of the compounds were all greater than 0.99, which fully meets the requirements detailed in method HJ759-2023. To verify the precision of the method and the stability of the instrument, the concentrations of 0.1 nmol/mol (low), 0.5 nmol/mol (middle), and 2.5 nmol/mol (high) standard gases were measured eight times. The peak area %RSD of all compounds was less than 7%, and the average %RSD value was 2.3%, as shown in Figure 8. The MDL was determined through eight replicate runs of a 0.1 nmol/mol standard gas. Under SIM mode, the MDL values of all compounds ranged from 0.002 to 0.013 nmol/mol, showing the ultrahigh sensitivity of this system. All the performance results are shown in Table 6.

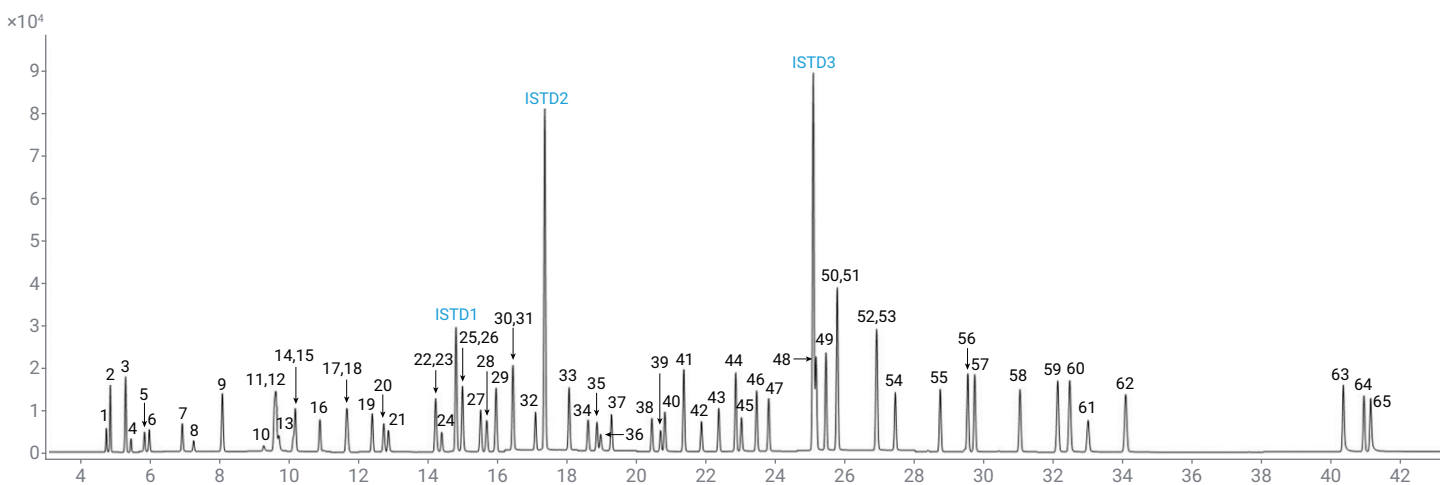


Figure 7. Total ion chromatogram of 65 VOCs at the concentration of 1 nmol/mol in SIM mode.

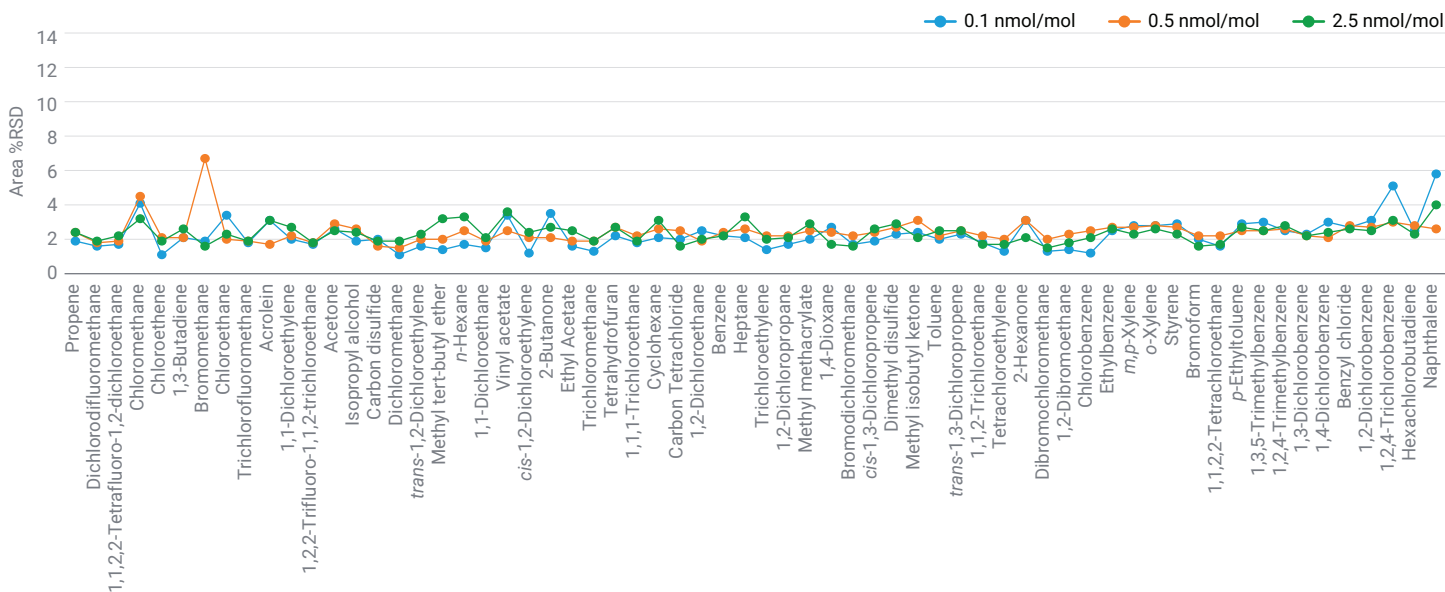


Figure 8. Repeatability results for 65 VOCs at low, middle, and high calibration levels in SIM mode.

Table 6. Linearity, repeatability, and MDL results for 65 VOCs in SIM mode (continued on the next page).

No.	Name	RT	RRF %RSD	CF2	Area %RSD			MDL (nmol/mol)	ISTD
					Low	Mid	High		
1	Propene	4.618	5.0	0.9999	1.9	2.4	2.4	0.004	1
2	Dichlorodifluoromethane	4.729	3.1	0.9999	1.6	1.8	1.9	0.002	1
3	1,1,2,2-Tetrafluoro-1,2-dichloroethane	5.171	2.5	0.9999	1.7	1.9	2.2	0.002	1
4	Chloromethane	5.46	16.0	0.9989	4.1	4.5	3.2	0.013	1
5	Chloroethene	5.725	2.8	0.9999	1.1	2.1	1.9	0.003	1
6	1,3-Butadiene	5.865	2.9	0.9998	2.1	2.1	2.6	0.004	1
7	Bromomethane	6.824	7.0	0.9998	1.9	6.7	1.6	0.004	1
8	Chloroethane	7.149	3.0	0.9998	3.4	2	2.3	0.007	1
9	Trichlorofluoromethane	7.947	3.0	0.9998	1.8	1.9	1.9	0.003	1
10	Acrolein	9.202	10.1	0.9998	3.1	1.7	3.1	0.012	1
11	1,1-Dichloroethylene	9.5	3.4	0.9999	2	2.2	2.7	0.003	1
12	1,2,2-Trifluoro-1,1,2-trichloroethane	9.532	2.9	0.9997	1.7	1.8	1.8	0.004	1
13	Acetone	9.654	21.6	0.9999	2.6	2.9	2.5	0.009	1
14	Isopropyl alcohol	10.081	9.3	0.9981	1.9	2.6	2.4	0.006	1
15	Carbon disulfide	10.105	5.8	0.9999	2	1.6	1.9	0.006	1
16	Dichloromethane	10.824	7.6	0.9998	1.1	1.5	1.9	0.004	1
17	trans-1,2-Dichloroethylene	11.597	3.5	0.9999	1.6	2	2.3	0.003	1
18	Methyl tert-butyl ether	11.648	5.5	0.9996	1.4	2	3.2	0.003	1
19	n-Hexane	12.35	18.5	0.9999	1.7	2.5	3.3	0.007	1
20	1,1-Dichloroethane	12.689	4.0	0.9996	1.5	1.9	2.1	0.002	1
21	Vinyl acetate	12.827	7.9	0.9996	3.4	2.5	3.6	0.008	1
22	cis-1,2-Dichloroethylene	14.177	4.0	0.9998	1.2	2.1	2.4	0.003	1
23	2-Butanone	14.221	5.1	0.9996	3.5	2.1	2.7	0.011	1
24	Ethyl Acetate	14.384	5.7	0.9997	1.6	1.9	2.5	0.005	1
25	Trichloromethane	14.966	3.4	0.9997	1.3	1.9	1.9	0.003	2

No.	Name	RT	RRF %RSD	CF2	Area %RSD			MDL (nmol/mol)	ISTD
					Low	Mid	High		
26	Tetrahydrofuran	15.005	5.7	0.9996	2.2	2.7	2.7	0.007	1
27	1,1,1-Trichloroethane	15.495	2.5	0.9999	1.8	2.2	1.9	0.005	2
28	Cyclohexane	15.665	3.5	0.9999	2.1	2.6	3.1	0.004	2
29	Carbon Tetrachloride	15.932	2.7	0.9998	2	2.5	1.6	0.005	2
30	1,2-Dichloroethane	16.428	8.1	0.9998	2.5	1.9	2	0.007	2
31	Benzene	16.428	6.0	0.9996	2.2	2.4	2.2	0.005	2
32	Heptane	17.079	3.0	0.9997	2.1	2.6	3.3	0.003	2
33	Trichloroethylene	18.041	3.4	0.9998	1.4	2.2	2	0.003	2
34	1,2-Dichloropropane	18.594	3.9	0.9998	1.7	2.2	2.1	0.004	2
35	Methyl methacrylate	18.867	6.7	0.9986	2	2.5	2.9	0.003	2
36	1,4-Dioxane	18.981	15.3	0.9913	2.7	2.4	1.7	0.008	2
37	Bromodichloromethane	19.265	3.4	0.9999	1.7	2.2	1.6	0.004	2
38	cis-1,3-Dichloropropene	20.437	4.8	0.9998	1.9	2.4	2.6	0.002	2
39	Dimethyl disulfide	20.684	10.0	0.9980	2.3	2.7	2.9	0.003	2
40	Methyl isobutyl ketone	20.83	9.1	0.9992	2.4	3.1	2.1	0.004	2
41	Toluene	21.36	5.5	0.9999	2	2.2	2.5	0.004	2
42	trans-1,3-Dichloropropene	21.87	6.2	0.9998	2.3	2.5	2.5	0.005	2
43	1,1,2-Trichloroethane	22.362	4.5	0.9997	1.8	2.2	1.7	0.005	2
44	Tetrachloroethylene	22.851	4.6	0.9997	1.3	2	1.7	0.003	2
45	2-Hexanone	23.04	9.7	0.9993	3.1	3.1	2.1	0.007	2
46	Dibromochloromethane	23.45	4.1	0.9999	1.3	2	1.5	0.003	2
47	1,2-Dibromoethane	23.801	4.1	0.9999	1.4	2.3	1.8	0.003	2
48	Chlorobenzene	25.161	4.4	0.9998	1.2	2.5	2.1	0.003	3
49	Ethylbenzene	25.447	5.4	0.9998	2.5	2.7	2.6	0.005	3
50,51	m,p-Xylene	25.767	9.2	0.9997	2.8	2.7	2.3	0.004	3
52	o-Xylene	26.897	8.9	0.9996	2.8	2.8	2.6	0.005	3
53	Styrene	26.921	13.1	0.9992	2.9	2.7	2.3	0.004	3
54	Bromoform	27.445	5.2	0.9999	2	2.2	1.6	0.004	3
55	1,1,1,2-Tetrachloroethane	28.731	3.3	0.9999	1.6	2.2	1.7	0.003	3
56	p-Ethyltoluene	29.528	11.7	0.9987	2.9	2.5	2.7	0.004	3
57	1,3,5-Trimethylbenzene	29.73	14.4	0.9988	3	2.5	2.5	0.005	3
58	1,2,4-Trimethylbenzene	31.03	13.4	0.9978	2.5	2.6	2.8	0.004	3
59	1,3-Dichlorobenzene	32.113	6.6	0.9999	2.3	2.2	2.2	0.003	3
60	1,4-Dichlorobenzene	32.459	7.6	0.9999	3	2.1	2.4	0.005	3
61	Benzyl chloride	32.993	13.4	0.9978	2.7	2.8	2.6	0.004	3
62	1,2-Dichlorobenzene	34.07	5.9	0.9999	3.1	2.7	2.5	0.006	3
63	1,2,4-Trichlorobenzene	40.318	12.0	0.9992	5.1	3	3.1	0.013	3
64	Hexachlorobutadiene	40.912	7.4	0.9997	2.5	2.8	2.3	0.006	3
65	Naphthalene	41.107	16.5	0.9978	5.8	2.6	4	0.012	3

Figure 9 shows the MDL results calculated under both scan and SIM modes. Compared to scan mode, the sensitivity results of SIM mode have improved by approximately 10x, which is consistent with the expectation. Therefore, if an analysis involves quantifying known trace components, SIM is a good choice to enhance sensitivity.

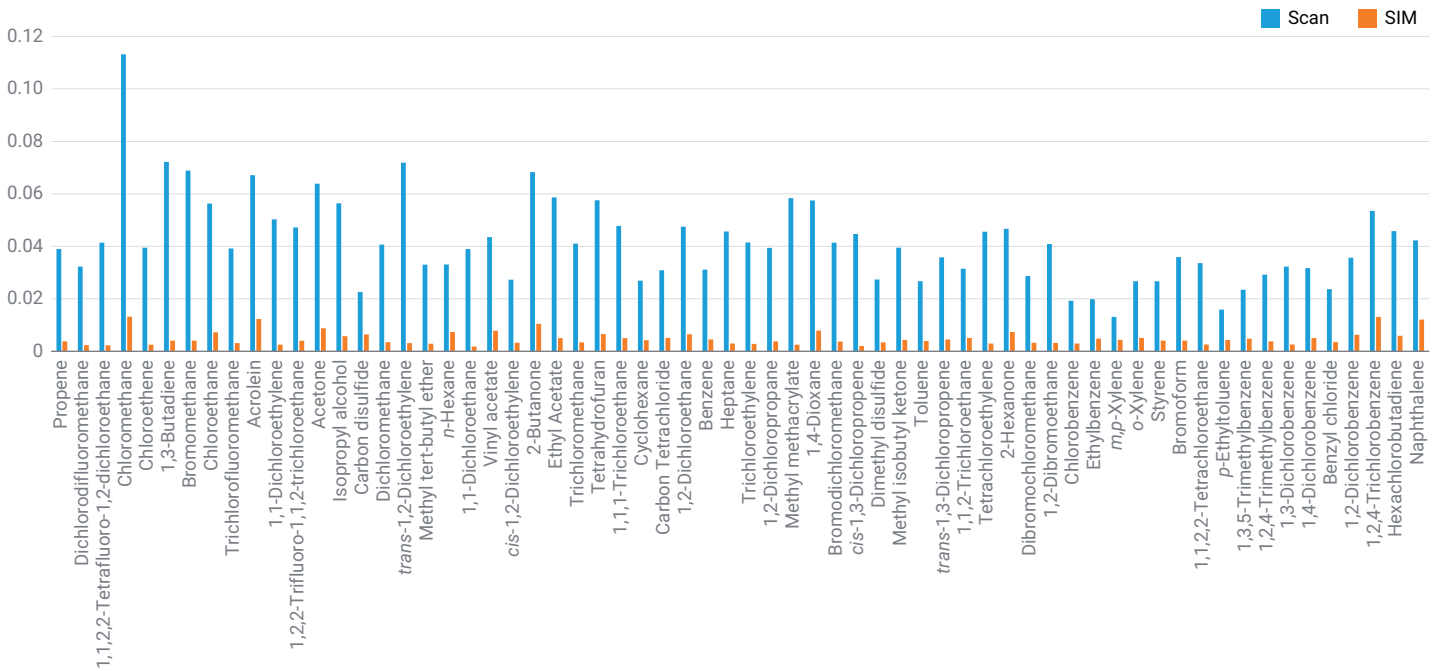


Figure 9. MDL results for 65 VOCs both in scan and SIM mode.

## Conclusion

An Agilent 8890/5977 GC/MSD system, equipped with a Multi-Gas CIA Advantage-xr TD provides a robust analytical procedure for the analysis of 65 VOCs in ambient air. This system offers a highly efficient and highly sensitive solution for the simultaneous analysis of multiple VOCs in both atmospheric quality monitoring laboratories and semiconductor cleanrooms. Based on different application requirements, users can choose to collect data in scan or SIM mode, demonstrating the flexibility of Agilent instruments. Excellent analytical performance has been achieved based on this system both in scan and SIM mode, which fully meets the requirements detailed in method HJ 759-2023.

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