

# Application News

GC-MS TD-30R/GCMS-QP2050

## Analysis of VOC and SVOC Emissions from Automotive Interior Materials Using GCMS-QP2050 in Accordance with ISO 12219-11

Masato Takakura, and Yuto Nakasuji

### User Benefits

- ◆ The GCMS-QP2050 features a new interface that enables good peak shape and sensitivity even when analyzing compounds with high boiling points.
- ◆ When used with the TD-30R thermal desorption system, it can analyze compounds in accordance with ISO 12219-11.
- ◆ The TVOC Calculation Tool can calculate in a simple manner quantitative emissions (toluene and hexadecane equivalents) in accordance with ISO 12219-11.

### Introduction

In recent years, measures to reduce the use of organic compounds in automotive interiors have progressed, the ISO 12219-11 standard is being developed for the analysis of volatile organic compounds (VOCs) and semi-volatile organic compounds (SVOCs) that are emitted from automotive interior materials. The ISO 12219-11 analytical procedure involves filling a thermal desorption (TD) glass tube with a sample of materials, heating the tube using TD, and loading the VOCs (up to C25) and SVOCs (C14 to C32) that were emitted from the sample into a GC-MS system for analysis. Although this standardized procedure enables simple and quick analysis of VOC and SVOC emissions from these materials, contamination of the MS system caused by the simultaneous loading of compounds with high boiling points is a problem.

As shown in Fig. 1, the GCMS-QP2050 is equipped with a new contamination-resistant ion optical system that effectively minimizes contamination of the MS. Featuring a new interface (Fig. 2) that enables good peak shape and sensitivity even for compounds that are typically prone to adsorption, it is optimally suited to analyzing SVOCs, including those with high boiling points.

TD-30R and GCMS-QP2020 NX will be listed as examples for suitable test equipment on ISO 12219-11. This Application News describes analyzing VOC and SVOC emissions from the materials of vehicle interiors in compliance with ISO 12219-11 using the GCMS-QP2050 together with the Nexis™ GC-2030 and the TD-30R thermal desorption system.



Fig. 1 GCMS-QP2050, Nexis™ GC2030, and TD-30R

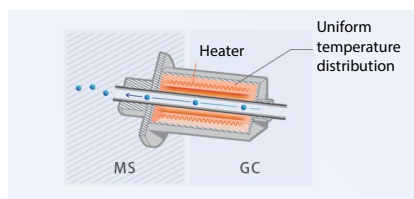


Fig. 2. Illustration of GCMS-QP2050's New Interface

### Equipment Configuration and Analytical Conditions

The analytical conditions used in this analysis are described in Table 1. The tube heating temperature was set at 280 °C for 20 minutes when measuring the calibration curve and control standard samples, and it was set at 90 °C for 30 minutes (VOC) and 120 °C for 60 minutes (SVOC), respectively, when measuring the emissions of test samples.

Table 1 Analytical Conditions

GC Model	: Nexis GC-2030
MS Model	: GCMS-QP2050 Entry
Autosampler	: TD-30R
[TD-30R]	
Tube Desorb Temp.	Standard: VOC : 280 °C (20 min) : SVOC : 90 °C (30 min) : 120 °C (60 min)
Tube Desorb Flow	: 82 mL/min
Trap Cooling Temp.	: -20 °C
Dry purge	: -20 °C, 82 mL/min, 1min
Trap Desorb Temp.	: 280 °C (10 min)
Joint Temp.	: 280 °C
Valve Temp.	: 280 °C
Transfer Line Temp.	: 280 °C
[GC]	
Injection Mode	: Split
Split Ratio (0 min – 3 min)	: 100
Carrier Gas Save Mode	: ON (Split ratio of 20 from 3 min after starting analysis)
Carrier Gas	: He
Carrier Gas Control	: Pressure (200 kPa)
Column	: SH-I-5Sil MS (P/N 227-36036-02) (60 m × 0.25 mm I.D., 0.25 μm)
Column Temp.	: 40 °C (3 min) – 10 °C/min – 300 °C (25 min)
[MS]	
TMP Evacuation Rate	: 60 L/sec
Ion Source Temp.	: 240 °C
Interface Temp.	: 280 °C
Acquisition Mode	: Scan
Event Time	: 0.5 sec
m/z Range	: 29 – 450
Tuning mode	: High Concentration

## ■ Analysis of Calibration Curve and Control Samples

The calibration curve standard samples were prepared by diluting toluene and n-hexadecane with methanol to concentrations of 0.5 µg/µL and then adding 4 µL of these respective samples to a Tenax TA collection tube. The analytical system's recovery rates were evaluated by preparing control standard samples of typical VOCs (a concentration of approximately 0.11 µg/µL) and adding 4 µL of each control sample to a Tenax TA collection tube for analysis. The response factors ( $R_f$ ) for toluene and n-hexadecane were calculated based on the measurement results for each calibration curve standard sample and Formula 1, which is shown below. As shown in Table 2, the calculation of control sample recovery rates that are based on toluene  $R_f$  indicated good recovery rates of 60 % to 140 % for each compound, including 80 % to 120 % for toluene. The total ion chromatograms (TIC Chromatograms) for the calibration curve samples and the control samples are shown in Fig. 3 and 4, respectively.

$$R_f = \frac{\mu\text{g (Toluene, C16)}}{\text{Peak area}} \times 1,000$$

Formula 1: Formula for calculating response factor ( $R_f$ )

Table 2 Control Sample Recovery Rates

Compound	Area	Recovery rate [%]
Benzene	835,986	77
n-Heptane	803,763	74
Toluene	1,082,965	100
n-Octane	907,774	84
p-Xylene	1,401,103	129
o-Xylene	1,382,117	127
n-Nonane	1,029,124	95
n-Decane	1,102,664	101
2-Ethylhexanol-1	1,014,840	93
n-Undecane	1,155,508	106
2,6-dimethylphenol	986,858	91
n-Dodecane	1,175,536	108
n-Tridecane	1,181,226	109
n-Tetradecane	1,156,078	106
Dicyclohexylamine	1,264,779	116
n-Pentadecane	1,104,602	102
n-Hexadecane	1,099,363	101
Di-(2-ethylhexyl)-adipate	945,870	87

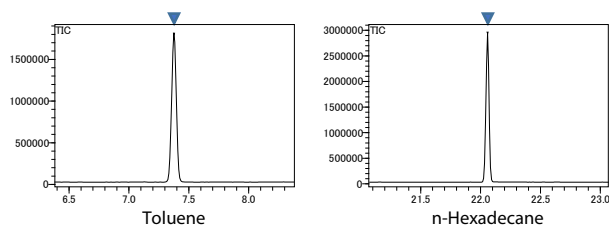


Fig. 3 TIC Chromatograms of Calibration Curve Sample

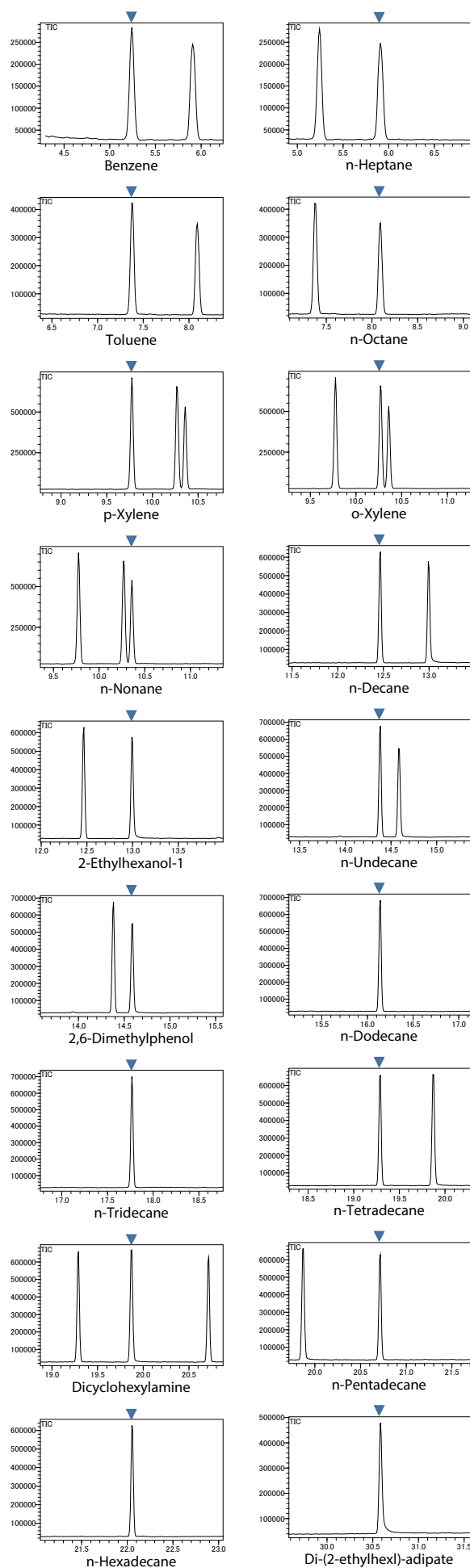


Fig. 4 Chromatograms of Control Sample

## ■ Tool for Calculating Toluene and Hexadecane Equivalents (TVOC Calculation Tool)

When analyzing samples according to ISO 12219-11, emission values for VOCs (up to C25) are calculated in toluene equivalents, and emission values for SVOCs (C14-C32) are calculated in hexadecane equivalents.

By simply importing the detected compound data and using the TVOC Calculation Tool, as shown in Fig. 5, the steps for calculating these equivalent emission values and generating reports can be automated.

### [ISO 12219-11 method for calculating emission values]

VOCs (from initial retention time to C25): calculated in toluene equivalents

SVOCs (C14-C32): calculated in hexadecane equivalents

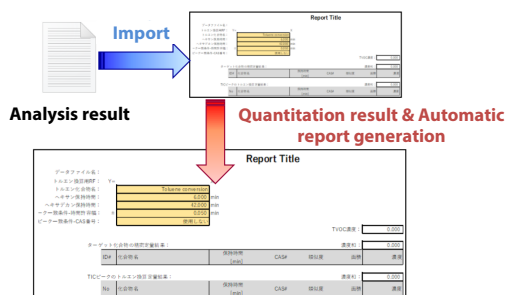


Fig. 5 TVOC Calculation Tool

## ■ Analysis of Automotive Interior Materials

A TD glass tube was filled with a sample of approximately 10 mg of thinly sliced leather materials taken from the interior of a vehicle. The sample was held in place by 5 mg of quartz wool inserted in both ends of the glass tube. Analyses of VOC and SVOC emissions were performed by heating the tube to 90 °C for 30 minutes and at 120 °C for 60 minutes, respectively, and measuring the emitted gases using the scan mode of the GCMS-QP2050. The TIC Chromatograms of VOCs and SVOCs that were emitted from the leather sample are shown in Figs. 6 and 7, respectively. The detected compound data were then imported into the TVOC Calculation Tool, and the VOC and SVOC emission values (µg/g) were automatically calculated (Figs. 8 and 9).

Using the TVOC Calculation Tool eliminates the inconvenience of having to manually calculate emission values according to Formula 2, which is shown below. These results can also be obtained by simply generating a report. Please refer to the TVOC Calculation Tool Manual for details.

$$\text{Emission } [\mu\text{g/g}] = R_f(\text{Toluene, C16}) \times \frac{\text{Peak area [counts]}}{1,000 \times \text{test portion sample } [\mu\text{g}]}$$

Formula 2: Formula for calculating compound emissions (µg/g) from automotive interior materials

Note: Before running the analysis, be sure to input the sample weight (mg) in the "sample quantity" parameter setting and the value of 1 in the "dilution factor" parameter setting in the LabSolutions™ GCMS batch file.

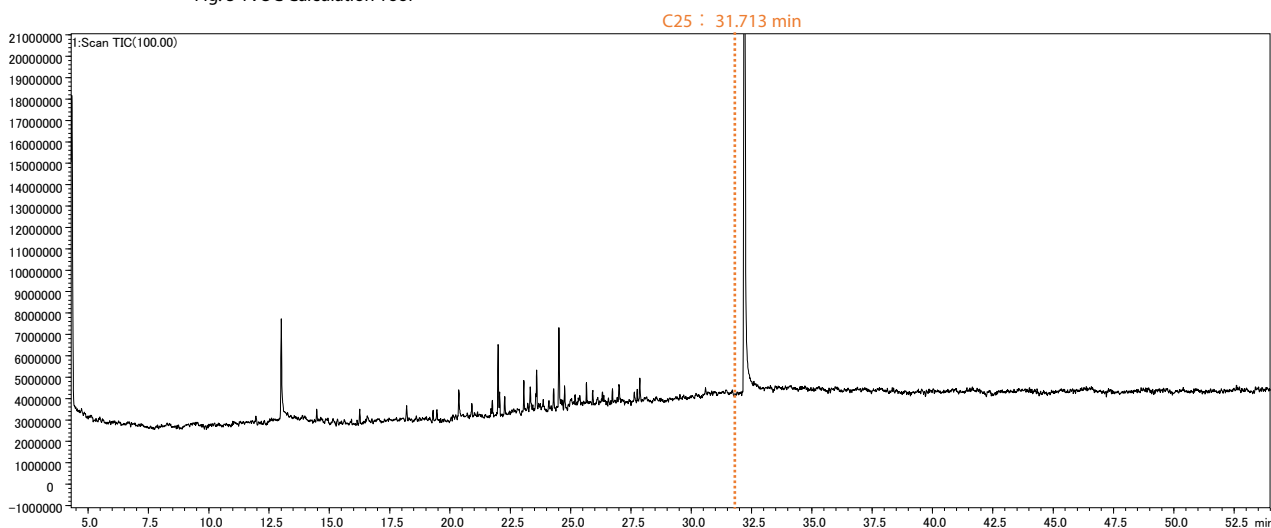


Fig. 6 TIC Chromatograms for VOCs

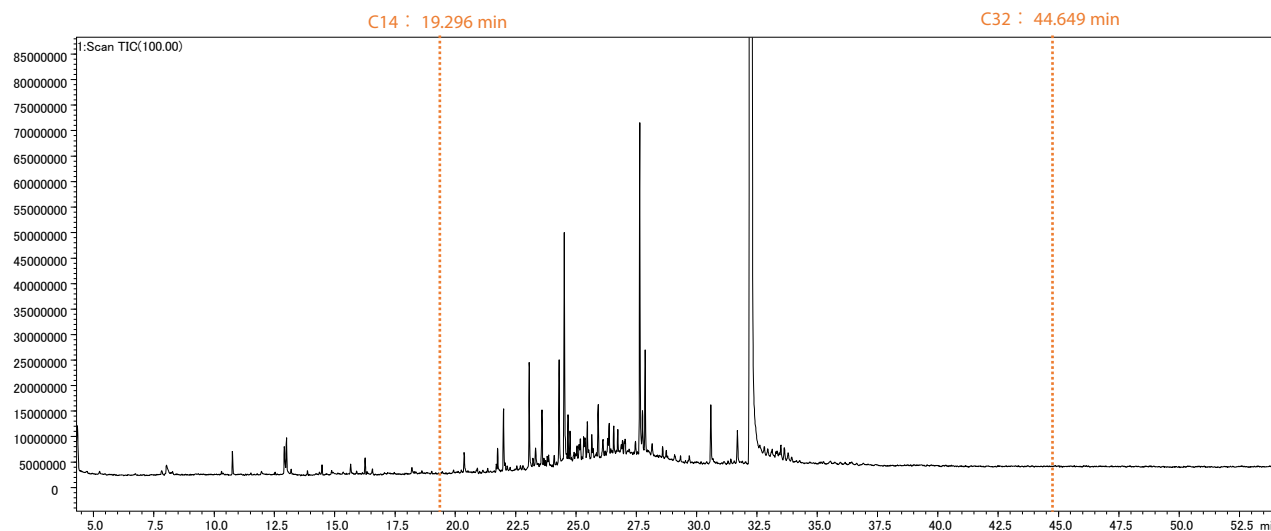


Fig. 7 TIC Chromatograms for SVOCs

### Analysis Results of VOC Emissions from Leather Materials (µg/g)

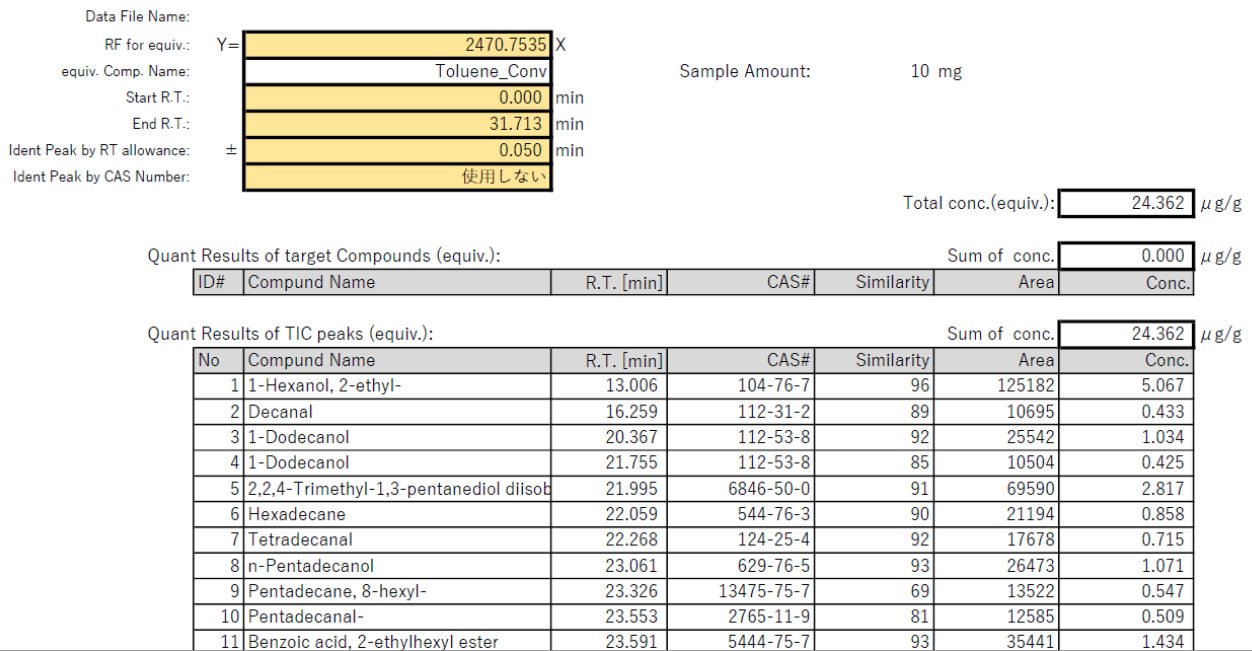


Fig. 8 Analysis Results of VOC Emissions from Leather Materials

Note: To set the equivalent  $R_p$ , select "Manual setting" and then input the inverse of the toluene  $R_p$  that was calculated with Formula 1.

### Analysis Results of SVOC Emissions from leather Materials (µg/g)

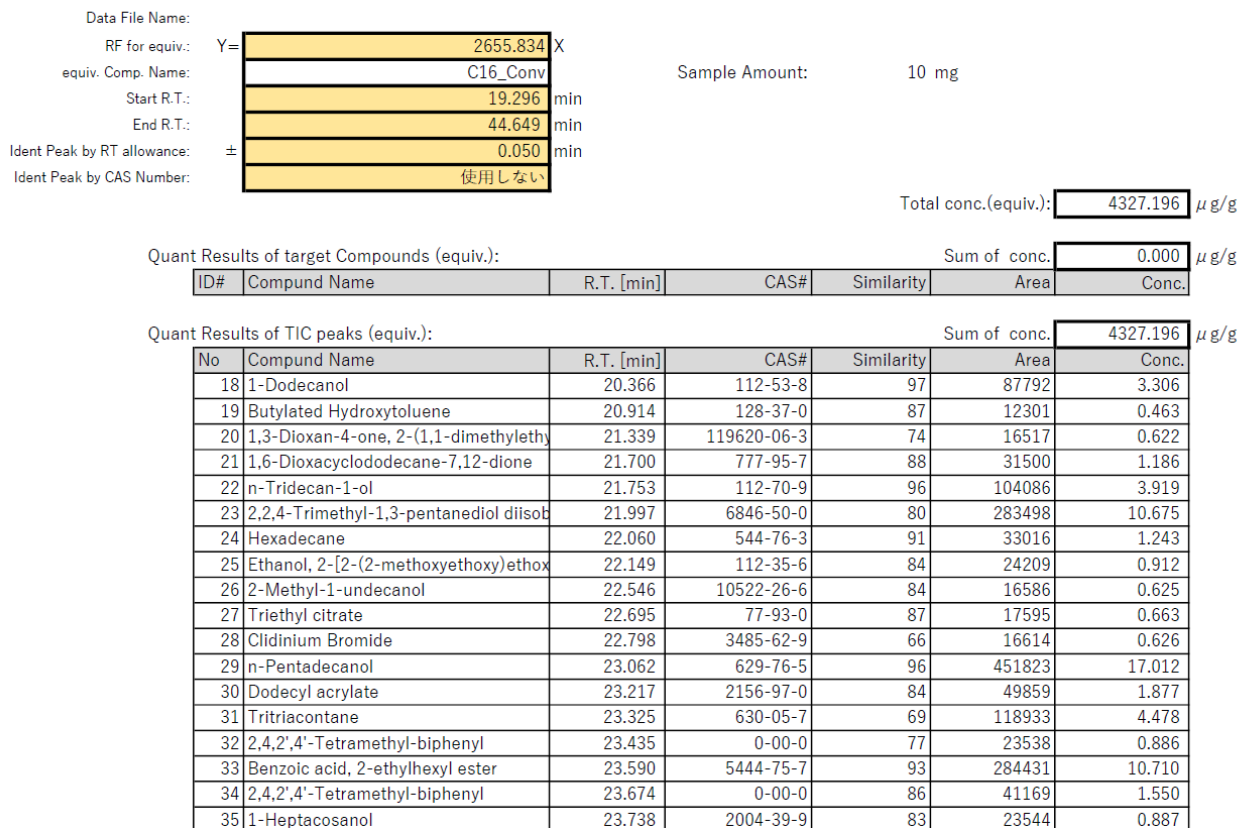


Fig. 9 Analysis Results of SVOC Emissions from Leather Materials

Note: To set the equivalent  $R_p$ , select "Manual setting" and then input the inverse of the hexadecane  $R_p$  that was calculated with Formula 1.

## ■ Conclusion

Using the new GCMS-QP2050, it was possible to consistently analyze SVOCs and other compounds with high boiling points. By combining this system with the TD-30R thermal desorption system and the TVOC Calculation Tool, even inexperienced users can rapidly analyze automotive interior materials and quantify emissions (i.e., calculate toluene and hexadecane equivalents) in compliance with ISO 12219-11.

Note: The TVOC Calculation Tool is optional software that is compatible with the new GCMS system models. Please contact a Shimadzu sales representative for details.

Nexis and LabSolutions are trademarks of Shimadzu Corporation or its affiliated companies in Japan and other countries.



# SHIMADZU

Shimadzu Corporation

[www.shimadzu.com/an/](http://www.shimadzu.com/an/)

**For Research Use Only. Not for use in diagnostic procedures.**

This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.

The content of this publication shall not be reproduced, altered or sold for any commercial purpose without the written approval of Shimadzu. See <http://www.shimadzu.com/about/trademarks/index.html> for details.

Third party trademarks and trade names may be used in this publication to refer to either the entities or their products/services, whether or not they are used with trademark symbol "TM" or "®".

Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The information contained herein is provided to you "as is" without warranty of any kind including without limitation warranties as to its accuracy or completeness. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication. This publication is based upon the information available to Shimadzu on or before the date of publication, and subject to change without notice.

01-00845-EN

First Edition: Jan. 2025

› Please fill out the survey

## Related Products

Some products may be updated to newer models.



### › GCMS-QP2050

Gas Chromatograph Mass Spectrometer



### › TD-30 Series

Thermal Desorption Systems

## Related Solutions

› Automotive

› Price Inquiry

› Product Inquiry

› Technical Service /  
Support Inquiry

› Other Inquiry