

Application Data Sheet

No.120

GC-MS

Gas Chromatograph Mass Spectrometer

Using a Method Translator Program for GC-MS Analysis with a Hydrogen Carrier Gas

Conventionally, helium gas has been used as the carrier gas in GC-MS analysis. However, due to the rapid rise in helium prices and delivery delays in recent years, hydrogen and nitrogen have been increasingly used as an alternative to helium. Due to characteristics that differ from helium, these gases cannot be used with existing analytical methods unless the methods are modified, which requires reevaluating method parameter settings specifically for these gases. In addition, in order to minimize a rise in background noise if hydrogen or nitrogen is used, a column with a narrower internal diameter is recommended. This results in significantly different elution times (retention times) for compounds and longer identification times compared to analyses when using helium.

This Application Data Sheet describes using the EZGC™ Method Translator program, supplied by RESTEK®, to translate a method that uses helium as the carrier gas into a method that uses hydrogen. It also compares the resulting chromatograms.

Translating the Analytical Method

In addition to changing the carrier gas from helium to hydrogen, EZGC™ Method Translator was used to change the column length from 30 m to 20 m and the internal diameter from 0.25 mm to 0.18 mm. Fig. 1 shows the parameter settings before and after translation. The various parameters are calculated based on the selected carrier gas and column. In addition to specifying the optimal gas flow rate and pressure, the program also translates the oven program based on the given settings. In this example, “Translate” was selected. This translates the method so that each compound is eluted in the same order as before translation.

Table 1: Analysis Conditions

GC-MS:	GCMS-QP2020
Column:	Rtx®-5MS (P/N 12623) (length: 30 m; 0.25 mm I.D.; df = 0.25 µm) Rxi®-5MS (P/N 13411) (length: 20 m; 0.18 mm I.D.; df = 0.36 µm)
Glass Insert:	Sky® Single Taper Inlet Liner with Wool (P/N 23336.5)
[GC]	
Injection Unit Temp.:	250 °C
Column Oven Temp.:	See Fig. 1
Injection Mode:	Splitless
High-Pressure Injection:	250 kPa (2.3 min)
Injection Volume:	2 µL
Carrier Gas Control:	Linear velocity (before translation) and constant pressure (after translation)
[MS]	
Interface Temp.:	250 °C
Ion Source Temp.:	230 °C
Ionization Method:	EI
Measurement Mode:	Scan
Scan Event Time:	0.3 sec
Scan Mass Range:	m/z 50 to 550

Confirm the required sensitivity and quantitation before purging lines with hydrogen gas. Due to the flammability of hydrogen gas, it must be handled very carefully. For information about appropriate safety measures, refer to the Shimadzu Corporation website.

<http://www.shimadzu.com/an/gc/support/faq/bombe/bombe1.html>

EZGC™ Method Translator

Carrier Gas

Original

Translation

Helium

Hydrogen

Column

Length

30.00

20.00

m

Inner Diameter

0.25

0.18

mm

Film Thickness

0.25

0.36

µm

Phase Ratio

250

125

Control Parameters

Outlet Flow

1.42

→

1.28

mL/min

Average Velocity

43.92

76.14

cm/sec

Holdup Time

1.14

0.44

min

Inlet Pressure (gauge)

→

99.80

101.02

kPa

▼

Outlet Pressure (abs)

0.00

0.00

kPa

Atm

Vacuum

Atm

Vacuum

Oven Program

ⓘ

Isothermal

ⓘ

Ramps

Number of Ramps

2 (1-4)

Ramp (°C/min)

Temp (°C)

Hold (min)

Ramp (°C/min)

Temp (°C)

Hold (min)

80

2

80

1.15

20

180

0

30.7

180

0

5

280

3

7.1

280

2.1

Control Method

Constant Pressure

▼

Results

Solve for

●

Efficiency

●

Speed

ⓘ

Translate

●

Custom

Run Time

30.00

20.59

min

Speed

1.46

x

Use FC Values for Original

Use FC Values for Translation

Fig. 1: Method Translator Screenshot

<http://www.restek.com/ezgc-mtfc>

Analytical Results Using a Translated Method

The methods before and after translation were used to measure a standard pesticide solution containing 70 components (0.1 mg/L) and an n-alkane mixture solution (C7 to C33, 5 mg/L). The parameters that remained the same before and after translation are shown in Table 1.

Total ion current chromatograms (TICC) for retention indices from about 1700 to 1800 are shown in Fig. 2. The correlation between retention indices before and after method translation for all 70 components is shown in Fig. 3. The elution order remained the same after translation. The retention times differed due to the changes in carrier gas and column dimensions, but the retention indices remained within ± 10 (within about 6 seconds) of the index prior to translation for all 70 components.

These results show that EZGC™ Method Translator can be used to translate methods into optimized methods with changed parameters, such as with the carrier gas changed to hydrogen, while also obtaining equivalent retention index values for compounds, even if a column with a different length or internal diameter is used. Consequently, the same retention indices can be used as before translation, which means the Automatic Adjustment of Retention Time (AART) function can be used after translation to easily correct retention times for target compounds and enable easy identification of components.

(For information about correcting retention times using retention indices, refer to the Shimadzu Corporation website:
<http://www.an.shimadzu.co.jp/gcms/gcmssol/sol1.htm>)

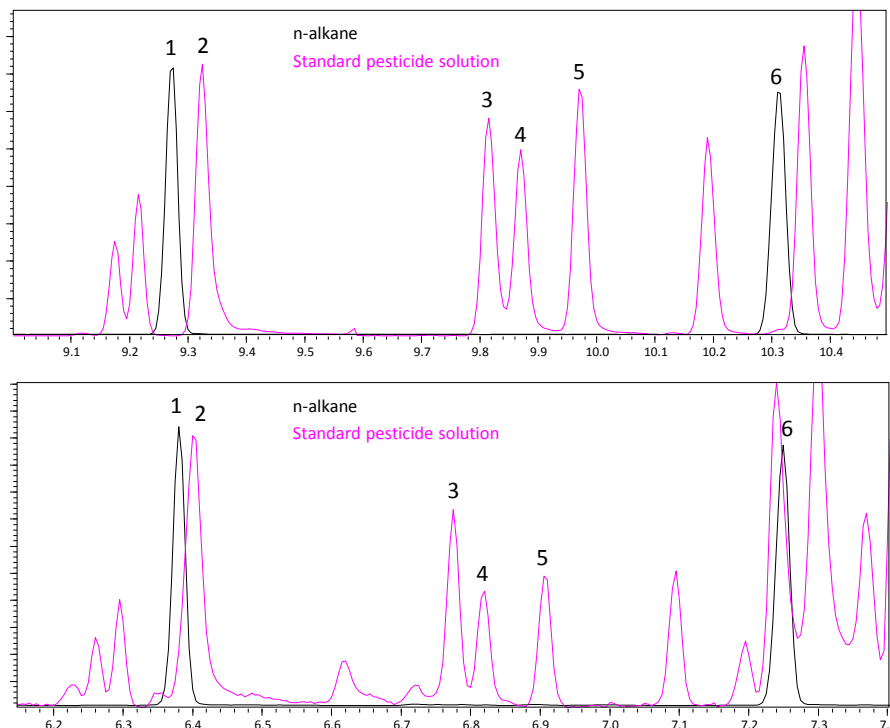


Fig. 2: TICC Before and After Method Translation (Upper: Before Translation; Lower: After Translation)

1. C17 (1700, 1700), 2. Pencycuron (1705, 1706), 3. Dimethoate (1753, 1747), 4. Simazine (1758, 1752), 5. Atrazine (1768, 1762), 6. C18 (1800, 1800)

Retention indices before and after translation are indicated in parentheses, in the form "(before, after)." Signal intensity was normalized based on peaks 1 and 2.

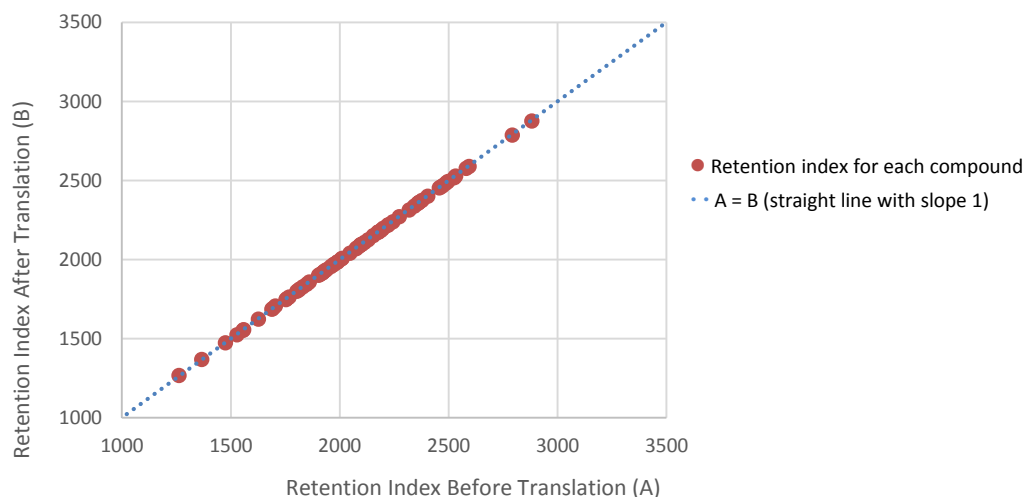


Fig. 3: Correlation between Retention Indices Before and After Translation

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