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Method conversion tool between instruments for huge-multiple MRM transitions in LC-MS/MS adopting the conversion factor of collision energy voltage

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Akane Yamamoto[1]; Kazutaka Ikeda[2]; Yoshiki Tainaka[1]; Jun Watanabe[1]
[1] Shimadzu Corporation, Kyoto, Japan;
[2] RIKEN Center for Integrative Medical Science, Yokohama, Japan

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Introduction

Triple quadrupole liquid chromatograph mass spectrometer (LC-MS/MS) has been used widely for targeted analysis in omics using huge-multiple MRM transitions and it is common that plural-manufacturers' mass spectrometers are owned and used in one laboratory. In this case, method transfer to one another instrument is often troublesome and difficult to validate their identity. Furthermore, optimal collision energy voltage in MRM transitions of each compound typically depends on the LC-MS/MS manufacturer.
In this study, we obtained the conversion factor of collision energy voltage from the correlation between the value of optimal collision energy voltage at one LC-MS/MS manufacture's instrument and that at another, and developed a tool to convert a method file from one to another using the conversion factor.

Methods and Materials

System

We used the date that ware performed using SCIEX LC-MS/MS (QTRAP 6500 and QTRAP 5500) and Shimadzu LC-MS/MS (LCMS-8060).

Figure1　LCMS-8060 triple quadrupole mass spectrometer (Shimadzu Corporation)

Methods

We picked up the value of collision energy voltage that was set for each compound from the method files of 58 compounds adjusted for SCIEX LC-MS/MS (QTRAP 6500 and QTRAP 5500) and Shimadzu LC-MS/MS (LCMS-8060), and compared them. As a result, it found that there was a correlation between collision energy voltage of each manufacturer and it did not depend on compounds. Therefore, by calculating the average ratio for the collision energy voltage that was set for each compound between above two manufactures, we obtained the conversion factor of collision energy voltage. Then, we developed a tool that automatically converted a method file of SCIEX software to that of Shimadzu software with adopting the conversion factor.

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Result

Result of collision energy voltage

We compared the optimized value of collision energy voltage that was set for each compound. The result is shown Figure 2.

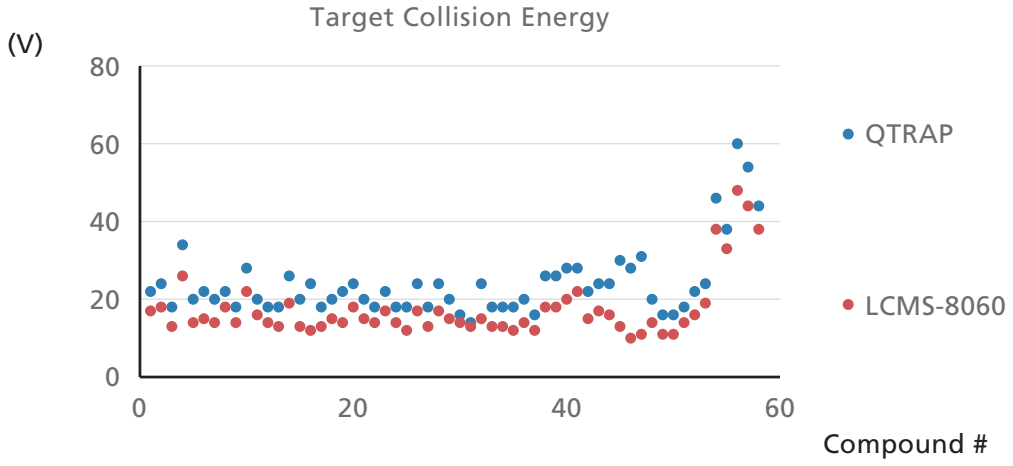

Figure 2 The correlation between collision energy voltage of each manufacturer

Figure 2 showed that there was a correlation between collision energy voltage of each manufacturer and it did not depend on compounds.
The correlation coefficient is 0.926.

We calculated the average ratio for the collision energy voltage that was set for each compound between manufactures. The result is shown Figure 3.

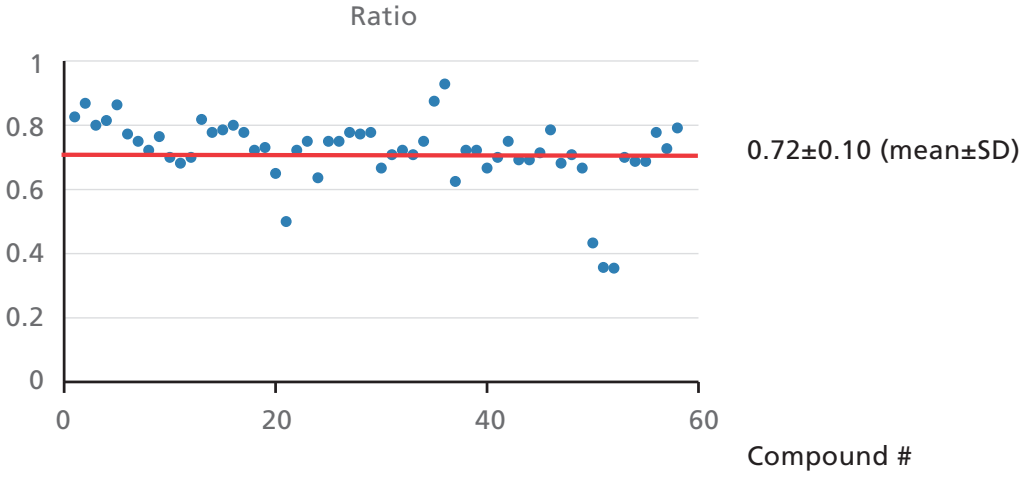

Figure 3 The ratio for the collision energy voltage

We obtained the average ratio “0.72” as the conversion factor of collision energy voltage from QTRAP to LCMS-8060.

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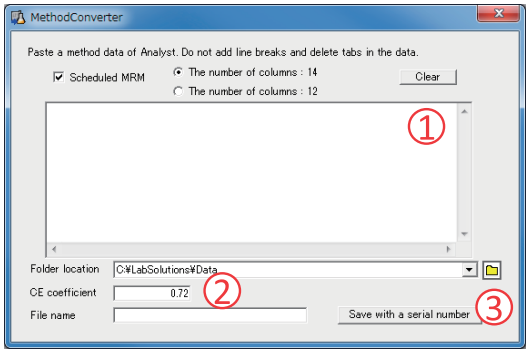
The tool details

We developed the conversion tool to convert a method of SCIEX software to a method of Shimadzu software (refer to Figure 4).



1. Method pasting field
2. Conversion factor setting box
3. Button outputting a converted method to a text file

Figure 4 The method conversion tool

In this study, the tool copies/converts the following parameters set in SCIEX.

Parameters to be copied :

- Compound Name
- Precursor ion m/z, Product Ion m/z
- Retention Time (only when Scheduled MRM is selected)

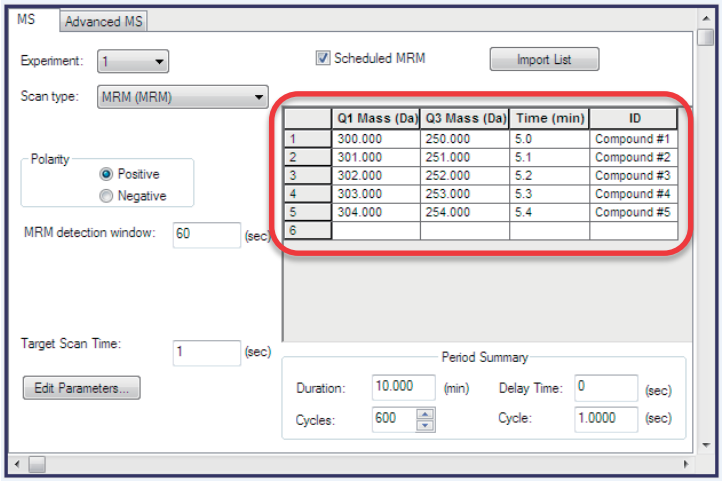
Parameter to be converted :

- Collision energy voltage

Note : Other than the above parameters are set to default value of Shimadzu software internally (e.g. Q1 Pre Bias).

The tool outputs in a text file the converted collision energy voltages for LCMS-8060 by adapted the conversion factor to the collision energy voltage set in a method file of SCIEX software. The tool also outputs the same MRM transition values (Precursor ion m/z, Product Ion m/z) and retention time in case of scheduled MRM. User should import the output text file to Shimadzu software.

Procedure are follows :



1. Copy MRM transition conditions (within a red frame in Figure 5) that were set in a method file of SCIEX analysis software and paste them to the tool (within a red frame in Figure 6).

Figure 5 The image of SCIEX analysis software

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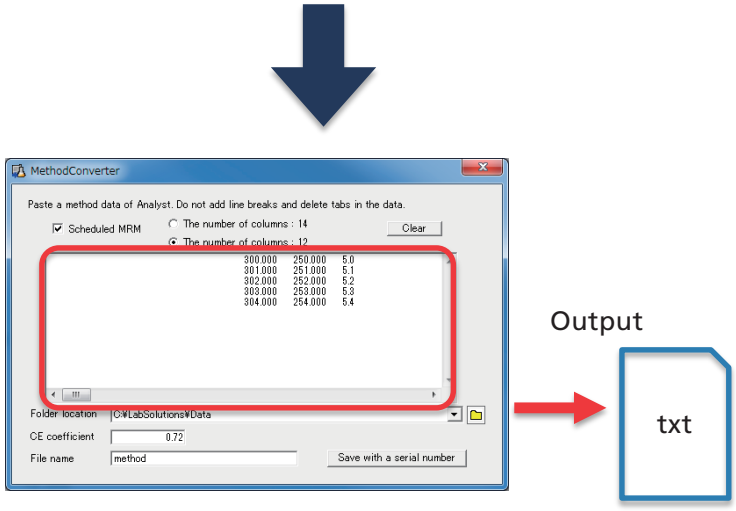

Figure 6 Text output image from the tool

2. Set (confirm) the conversion factor of collision energy voltage (default value “0.72” is preset) and the file location in which converted text file will be created.
3. Click the outputting button.

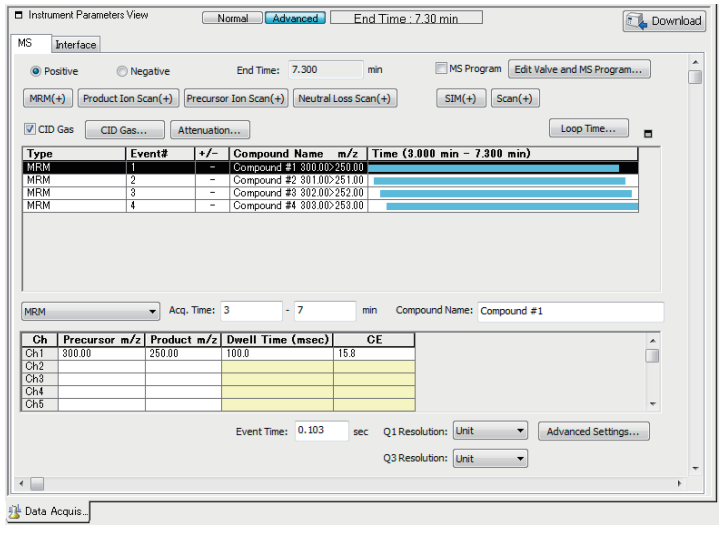

Figure 7 Shimadzu software after importing the method

4. Import the output text file to Shimadzu software and save as a new method.

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Analysis results obtained by using the converted methods

The data analyzed with QTRAP using the method before conversion and those with LCMS-8060 using the method after conversion with this method conversion tool are shown below (Figure 8).

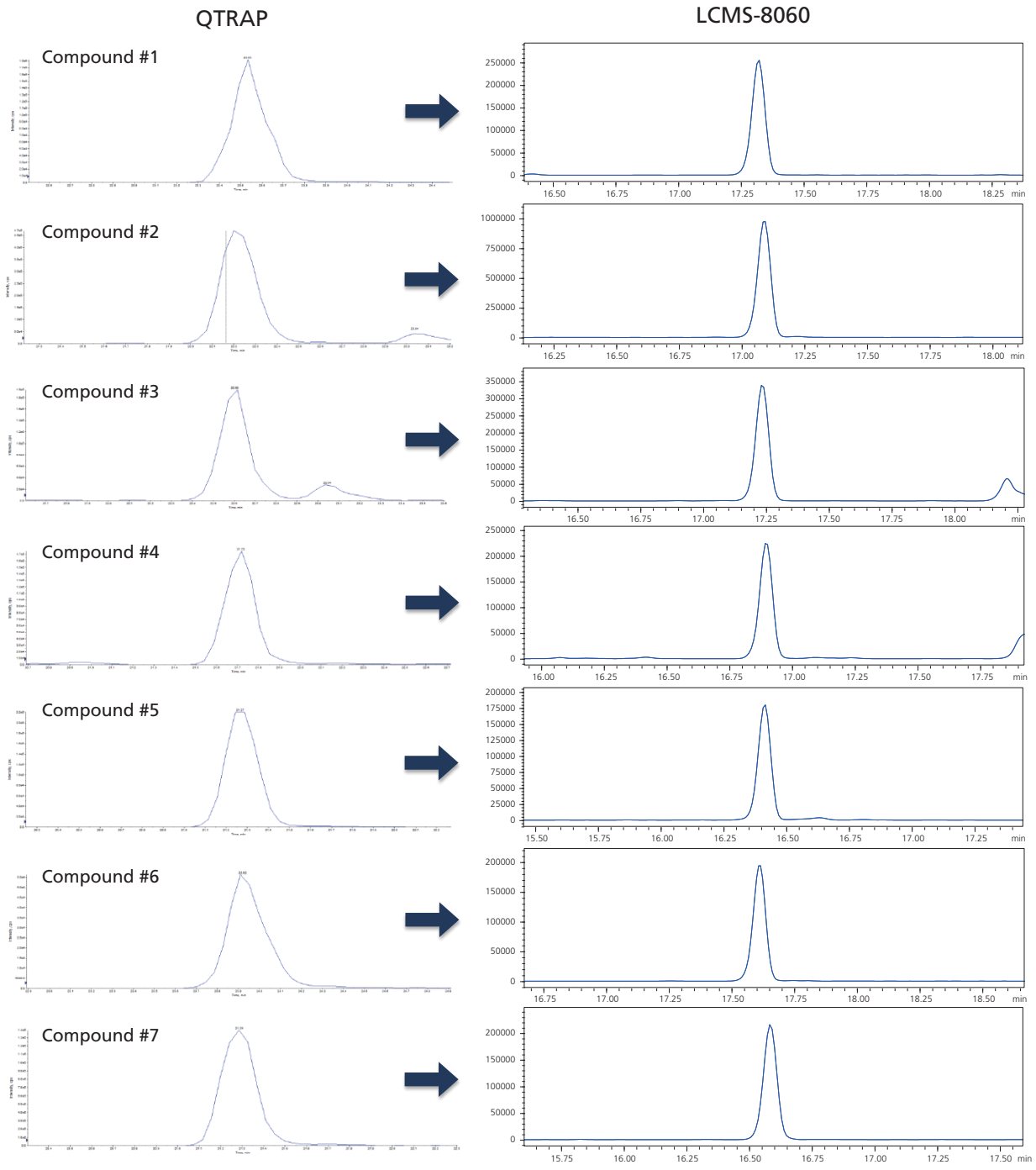

Figure 8 The results of QTRAP and LCMS-8060

Same peaks could be detected by using the converted method files.

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Conclusions

- We identified the conversion factor of optimal collision energy voltage, and developed a method conversion tool.
- With the converted method files, we could detect same peaks as with method files before conversion.

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