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Application Data Sheet

No.98

GC-MS
Gas Chromatograph Mass Spectrometer

Automatic Optimization of Transitions and Collision Energies

In GC-MS/MS MRM mode, the optimal transitions (combinations of precursor ion and product ion) and collision energies (CEs) must be determined. However, optimizing transitions can be difficult when analyzing many compounds. GCMSsolution (ver. 4.20 and later) control software for the GCMS-TQ series is equipped with an MRM optimization tool. This Data Sheet introduces the procedure for optimizing transitions using the MRM optimization tool.

Procedures for Optimization of Transitions

Transition is a combination of product ion and precursor ion. For MRM analysis, the best combination of product ion and precursor ion must be determined.

About transition
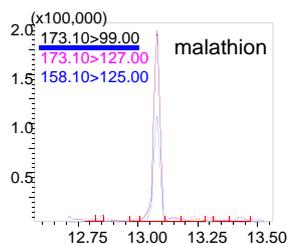
Let's take a look at the MRM chromatogram of malathion as an example. Transition is "173.10>99.00", "173.10" is Precursor ion, "99.00" is Product ion.

■Elements of MRM analysis
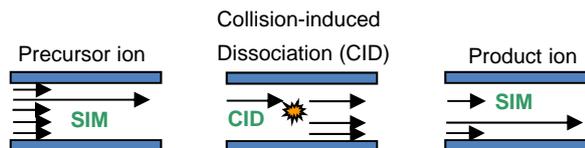
Precursor ion: When other ions are generated from one ion, Precursor ion is the original ion. Same as the parent ion.

Product ion: Product ion is generated from the certain ion. Original ion is the Precursor ion, same as the daughter ion.

Optimization of the transitions consists of four steps (below). Using the MRM optimization tool, only analyzing the data acquired in the Scan mode, allows optimizing the transition automatically.

Step 1 Analyze Data in Scan Mode

Step 2 Create a Method File for Product Ion Scan Mode

Step 3 Collect Data in Product Ion Scan Mode

Step 4 Determine the Transitions and Their Optimal CEs

| manual | Auto | Auto | Auto |

Step 1：Analyze Data in Scan Mode

Run the GCMS Postrun program. Display the data file collected in Q3 Scan mode.
Check that the compounds are identified correctly.
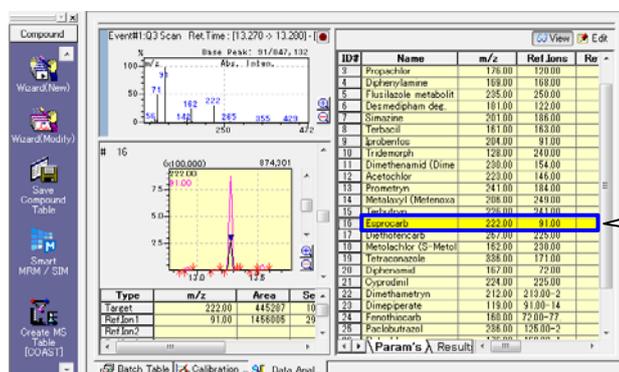
The compound masses and confirmation ions are configured to the precursor ions. With the MRM optimization tool, you can optimize transitions using multiple precursor ions for each compound.

Step 2：Create a Method File for Product Ion Scan Mode

After confirming the compounds are identified correctly, click the [icon] icon.
An MS table is created automatically.
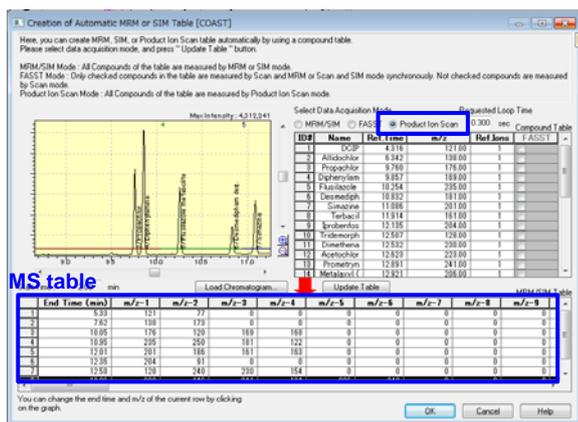
Select [Product Ion Scan]; an MS table is then automatically created. The created table can be corrected while checking the chromatogram. If no problem exists in the MS table, a method file for Product Ion Scan Mode is created

Step 3：Collect Data in Product Ion Scan Mode
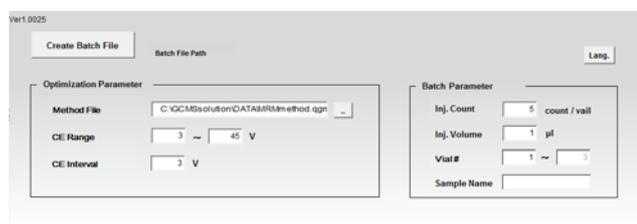
To use the MRM optimization tool, just set the parameters shown in the figure on the left to automatically create multiple method files (product ion scan mode) and batch files with the CEs configured. Using the batch file, start a consecutive product ion scan analysis.

Step 4：Determine the Transitions and Their Optimal CEs

Transitions can be optimized to select the data files obtained through measurements using the MRM optimization tool. Fig. 1 shows the graph of transitions and CEs. CEs were optimized with high accuracy.
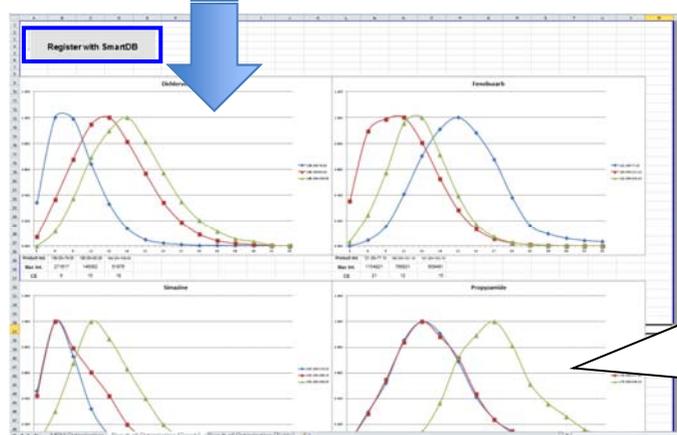
Utilizing high-speed scan control technology, the GCMS-TQ series allows a simultaneous product ion scan analysis of multiple components. As shown in Fig. 1, even if you had optimized the CEs and transitions in the simultaneous analysis, CEs could be optimized with high accuracy. This is useful when optimizing multicomponent transitions, such as when migrating to GC-MS/MS from GC-MS methods.

Fig. 1: Component Transitions and CEs

The optimized transitions can be registered in Smart Database. With Smart Database, you can automatically create MRM analysis methods using the transitions and CEs determined with the MRM optimization tool. For the procedure for creating MRM analysis methods, see Application Data Sheet No. 97.

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