

Application News

No. C163

Liquid Chromatograph Mass Spectrometry

MRM Database of 836 Residual Pesticides for LabSolutions Connect and Insight

Multiple Reaction Monitoring (MRM) is the standard method of data acquisition for high sensitivity Triple Quadrupole LC-MS/MS analysis. Each MRM precursor ion and product ion pair represents a specific fragmentation transition for a given molecule. For even more specificity, multiple MRM transitions are often monitored for each analyte. Establishment of accurate MRM transitions requires the analysis of an authentic standard under a range of voltages to optimize sensitivity. Shimadzu's LC-MS/MS Method Package for Residual Pesticides Ver. 3 is a data base containing multiple pre-optimized MRM transitions for 836 pesticides, including chromatographic conditions.

These 836 pesticides represent a combination of several world-wide regulatory lists, including the Japanese Ministry of Health, Labour and Welfare (MHLW) positive

list system, Regulation (EC) No 396/2005 of the European Parliament and of the Council, and China's food safety national standards regulations (GB standards).

LabSolutions Connect easily creates MRM methods for any of these lists or any combination of analytes.

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Method Creation and Batch Analysis Using LabSolutions Connect

Four simple steps to create an MRM method and set up a batch acquisition table are shown in Figure 1 below. In this example, a method template for the analysis of GB standards is chosen, and a batch table is created for the analysis of a calibration curve.

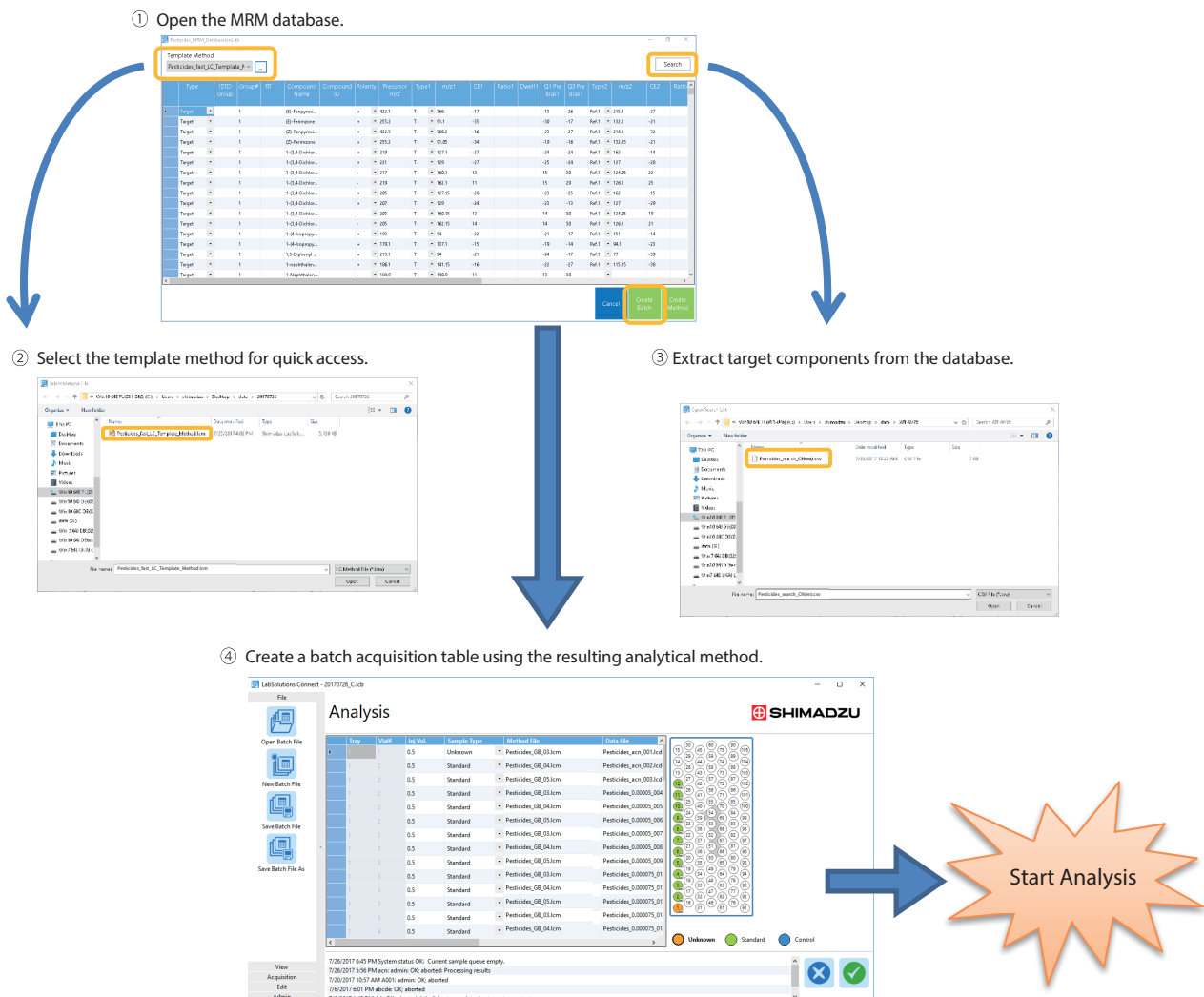


Fig. 1 Sequence for Method Creation and Batch Analysis Using LabSolutions Connect

■ Data review using LabSolutions Insight

MRM methods are suitable for the simultaneous analysis of hundreds of different compounds in a single chromatographic run. This means that thousands of individual MRM chromatograms can be acquired by a typical laboratory in a single day. A software solution is required to speed up data processing and achieve faster turnarounds for the laboratory.

Shimadzu's LabSolutions Insight is data review software designed to streamline complex laboratory workflows and dramatically improve productivity. LabSolutions Insight has powerful data mining and analytics capabilities for reviewing multi-analyte LC-MS/MS results. The clear, intuitive interface is designed to support review-by-exception, enabling quality rules to identify exceptions quickly. Insight automatically applies your chosen criteria

to data and flags any deviations, allowing you to immediately identify and analyze them.

Shimadzu's Ultra-Fast LC-MS/MS technologies are capable of acquiring hundreds of chromatographic peaks in just minutes. In the Figure 2 below, an MRM chromatogram for fenobucarb is shown. This pesticide eluted between 5.5 and 5.7 minutes, along with 40 other compounds in the same narrow window. MRM dwell times of just 1 msec enabled adequate peak shape and a detection limit of 0.5 ug/L, ten times lower than the GB standards regulatory limit.

LabSolutions Connect and LabSolutions Insight provide a seamless workflow to establish MRM methods and review the complex results. Laboratories will benefit from easy MRM selection and streamlined data analysis, taking full advantage of Ultra-Fast LCMS technologies from Shimadzu.

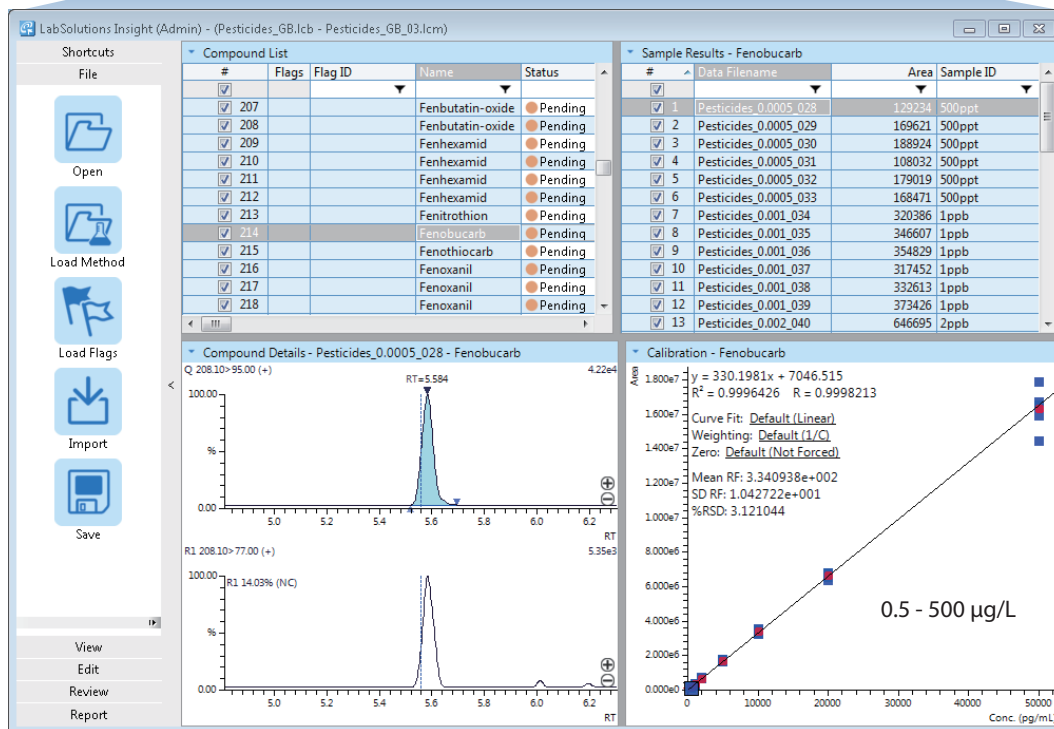
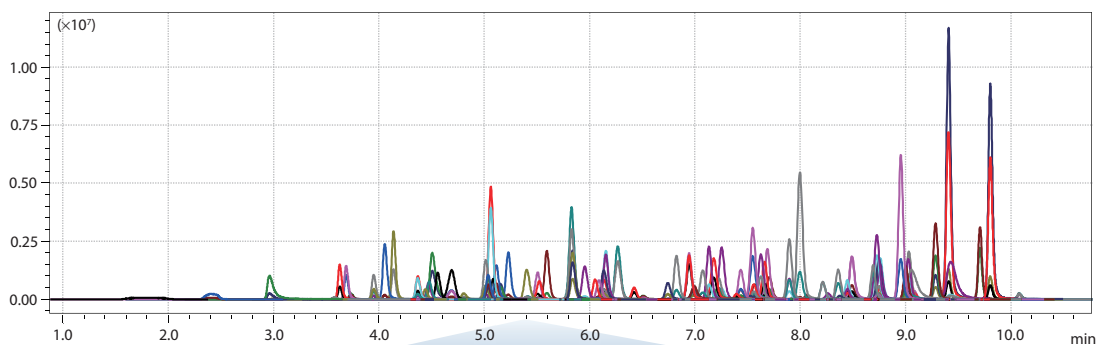


Fig. 2 LabSolutions Insight Data Review of Fenobucarb MRM Chromatograms and Calibration Curve

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