

GC-MS/MS Analysis Made Easy with Xevo TQ-GC and Quanpedia Database

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GOAL

Learn how Quanpedia™ Database can simplify GC-MS/MS method development and analysis in food and environmental laboratories.

BACKGROUND

Generating multiple reaction monitoring (MRM) transitions for GC-MS/MS analyses which cover a wide range of target compounds can be a time-consuming challenge. Laboratories often have to generate these methods or regularly update existing methods to meet regulatory and customer demands. This method development process is not only time-consuming, but it also requires expert knowledge of compounds and the use of expensive standards. Traditionally, the use of product ion scans at various collision energies has been implemented to generate MRM transitions. This is a very manual process that is susceptible to user error. Even utilizing existing method information of MRM transitions collated in spreadsheets could introduce transcription errors. Waters™ Xevo™ TQ-GC is enabled with Quanpedia, a compound-centric GC EI MRM database that acts as a starting point to reduce

Use Quanpedia Database to rapidly build GC-MS/MS methods.

The screenshot displays the Quanpedia software interface with several key components and callouts:

- Select Analysis:** A panel on the left allows users to select an analysis from a list. A callout box states: "Select a pre-existing method or generate a customized method".
- Select Compounds:** A panel at the bottom allows users to select one or more compounds from an available list. A callout box states: "Automatically generate GC and MS acquisition methods and processing method".
- Acquire data:** A central panel shows the acquisition parameters and a callout box states: "Acquire data".
- Reviewable results:** A panel on the right displays the resulting chromatogram and mass spectra. A callout box states: "Reviewable results with minimal method development".

Figure 1. Overview of Quanpedia workflow.

method development time. Customized GC-MS/MS methods can be created or modified quickly as required.

THE SOLUTION

Quanpedia employs a compound-centric database that holds GC chromatographic conditions, MRM transitions, and TargetLynx™ quantitation information all in one place. Information may be imported from existing methods, third-party files, or supplemented manually. Compounds can be searched within the database to retrieve compound specific MRMs to drive analytical method development. MRMs can also be imported easily into the Quanpedia Database from legacy methods. Retention times for all of the compounds in each method can be updated within Quanpedia to compensate for any shifts in retention times due to column maintenance. The Quanpedia functionality for the Xevo TQ-GC is exactly the same as that of the Xevo tandem quadrupole -MS product lines. This reduces the need for training users who already use Waters' Xevo TQ-MS systems.

SUMMARY

Use the Quanpedia Database to quickly generate GC-MS/MS methods without the need for manual input of MRM transitions, GC methods, or data processing methods. Quanpedia covers a wide range of key compounds of concern for food and environmental contaminant testing labs. By considerably simplifying GC-MS/MS analysis and having a compound centric database containing over 1000 compounds, lab productivity can be increased.

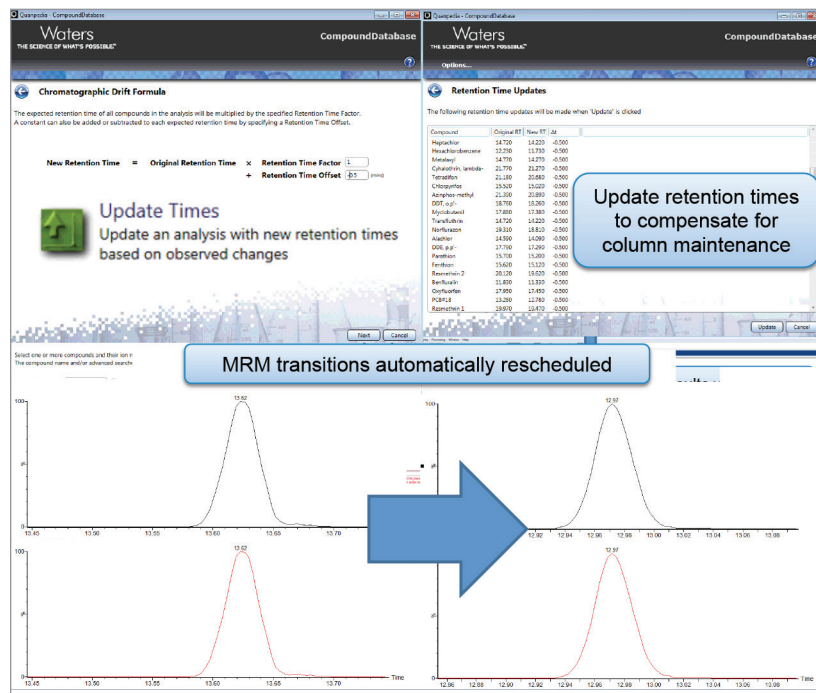


Figure 2. Adjustment of the retention times for the entire GC-MS/MS method within the Quanpedia Database.

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