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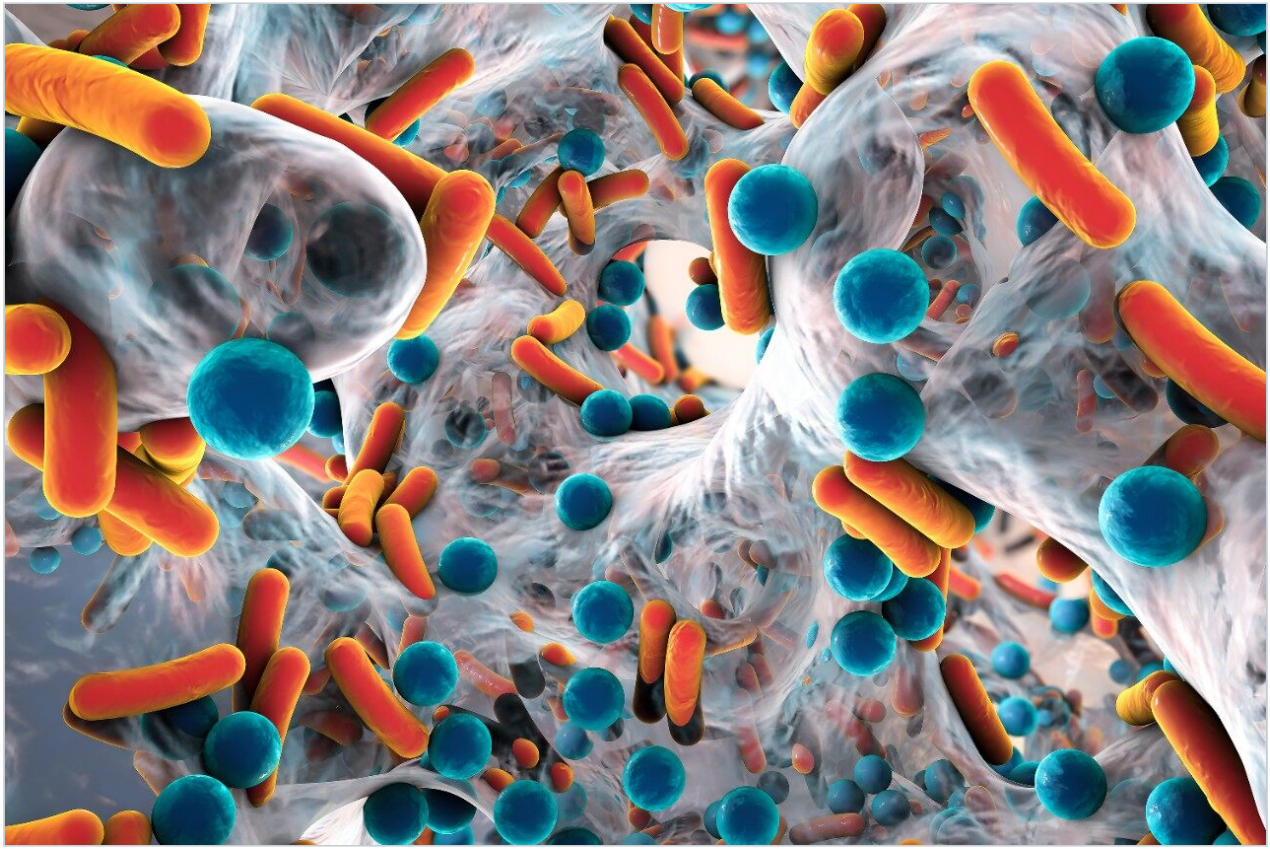
응용 자료

Quanpedia Database: A Compendium of Compounds and Analyses for Rapid and Simple Multi- Residue LC-MS/MS Method Development

Waters Corporation



This is an Application Brief and does not contain a detailed Experimental section.

Abstract

In this technology brief, we demonstrate the functionality of Quanpedia database for rapid and easy access to chromatographic, MS acquisition, and processing methods for the development of analytical methods.

Benefits

Quanpedia is an extensible and searchable database for quantitative UPLC/MS/MS analytical method development

Introduction

LC-MS/MS analysis requires LC, MS, and quantification methods in order to acquire and analyze data. Quanpedia is a “one-stop” central database for quantitative as well as qualitative LC-MS method information. Quanpedia employs a compound-centric database that holds all UPLC chromatographic, MS/MS acquisition, and TargetLynx quantification information in one place. At present, Quanpedia has over 40 pre-defined analyses with information on over 1,000 compounds for LC-MS/MS analysis. For example, existing methods are available for the following groups: veterinary drugs, antibiotics (including nitrofurans and associated metabolites), hormones, amphetamines, mycotoxins, pesticides, water soluble vitamins, and other compounds, such as melamine resin. Quanpedia also offers users the option to append their own methods and compounds and the ability to modify or update existing methods to build a customized, evolving scientific database.

Quanpedia acts as a comprehensive repository of information related to a Selected Ion Reaction (SIR) or Multiple Reaction Monitoring (MRM) analysis for a given compound. By simply selecting compounds from the database, Quanpedia automatically creates both data acquisition methods and the associated data processing methods required to perform the analysis.

Quanpedia enables efficient, rapid, and easy information management of both methods and compounds, allowing new methods to be rapidly generated for any of the compounds contained within the database. Compound and method information can easily be shared between multiple workstations or laboratories, thus reducing the risk of transcription errors.

In January 2012, the presence of the banned pesticide, carbendazim in imported orange juice was reported.

In order to efficiently screen orange juice consignments for carbendazim and other residues, a multi-residue analytical method incorporating 401 pesticides and associated acquisition and processing methods was set up using the Quanpedia database. The simplicity of the method development process is demonstrated in this technology brief.

Results and Discussion

A multi-residue pesticide analytical method applicable for the screening orange juice samples was developed. The pre-defined Pesticide Screening analysis was selected from the Run Samples menu within the Quanpedia database. The analysis provided the UPLC method conditions and two MRM transitions for each of the 401 pesticides. A screenshot highlighting the automated scheduling of the MRM transitions for the targeted pesticides obtained from Quanpedia is shown in Figure 1. The MS method, including the appropriate retention time windows, was generated in seconds. In addition to the LC and MS conditions, the TargetLynx data processing method for all 401 pesticides was also generated.

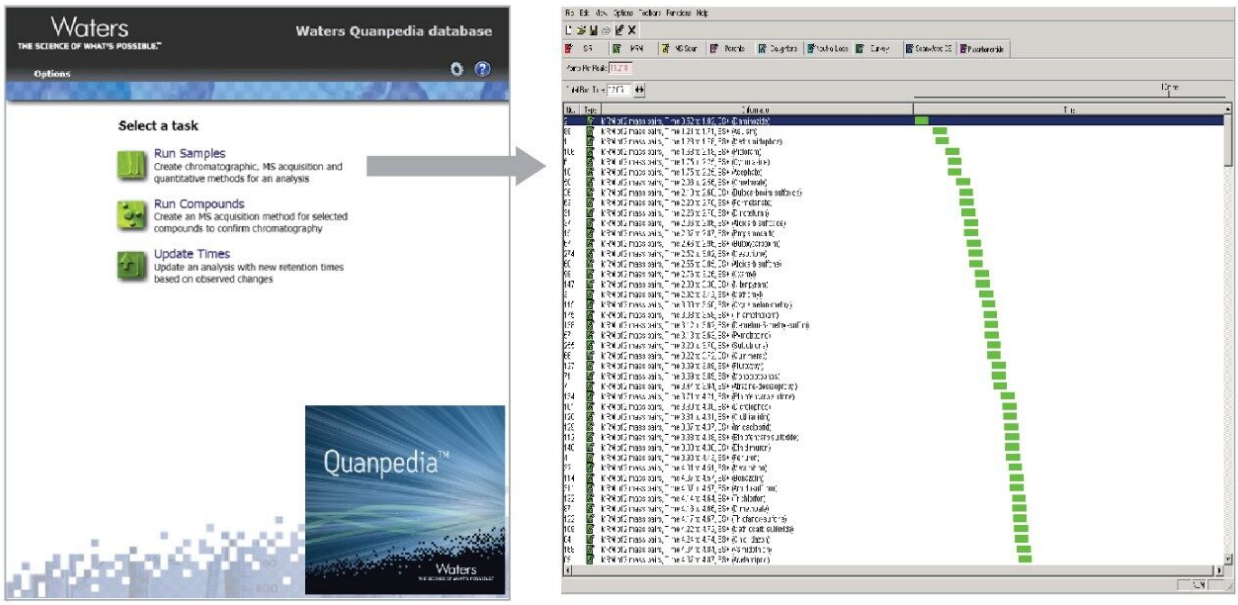


Figure 1. Screenshot of a portion of the MRM transitions for 401 pesticides obtained from Quanpedia.

An alternative approach to LC-MS/MS method development is to select the specific compound(s) of interest and generate a more limited analytical method. However, when analyzing a sample that may contain many

pesticides, the multi-residue screening approach was deemed to be more informative. Due to the enhanced sensitivity of the Xevo TQ-S Mass Spectrometer and its rapid electronics, performing multi-residue analysis within a single injection is possible without compromising the data quality.

Using the LC-MS/MS method obtained from Quanpedia, samples of orange juice were analyzed using the ACQUITY UPLC I-Class System coupled to the Xevo TQ-S Mass Spectrometer. An orange juice sample, previously tested and shown to be free from the 401 pesticides, was spiked with a mix containing 80 pesticides each at 10 ng/mL. The spiked juice sample was then diluted 100 times with water and filtered using 0.45 µm syringe filter followed by direct injection onto the column.

Figure 2 shows the MRM chromatograms of three pesticides which eluted between 9 to 10 min. In total, 89 pesticides were found to elute in this narrow region of the chromatogram using the selected method. With the ability to quickly generate acquisition windows around the retention time of each individual pesticide and automatically calculate the required dwell times (AutoDwell), the data generated is of the highest achievable quality. Even with the large number of transitions and closely eluting peaks, a minimum of 10 data points were obtained across each peak, ensuring accurate quantification and a high level of repeatability.

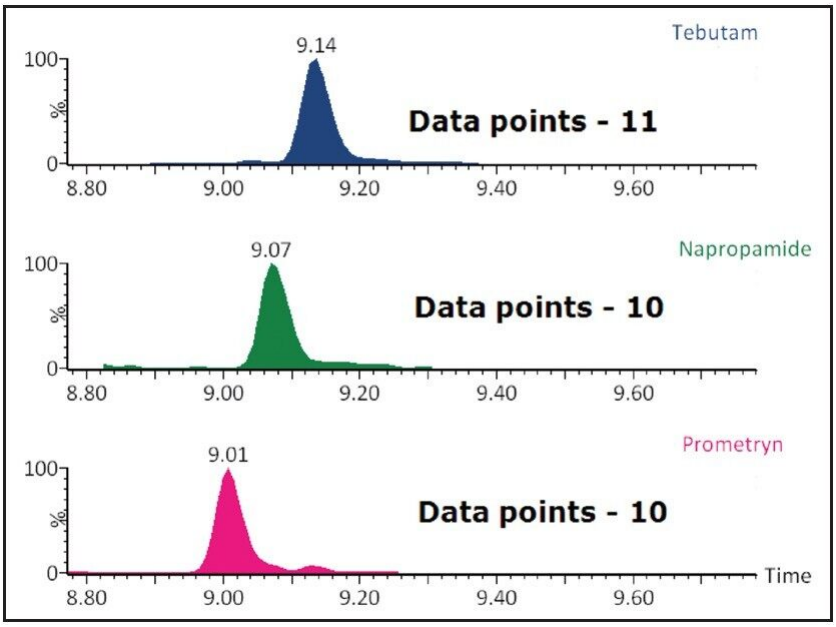


Figure 2. MRM chromatograms of three different pesticides at 10 ng/mL in orange juice.

Conclusion

Quanpedia is an extensible and searchable database for quantitative UPLC/MS/MS analytical method development. Quanpedia for MassLynx Software has been developed as part of Waters integrated workflow innovations for analytical chemical laboratories.

Quanpedia enabled the rapid generation of acquisition and processing methods for the simultaneous analysis of multiple pesticide residues following a recent report of the detection of a misused fungicide. The use of optimized acquisition time windows around each compound's retention time and automatic selection of the appropriate dwell time ensured the highest quality data and most accurate quantification. The application of Quanpedia is easily extended to other compound types included in the database and ensures transferability of methods within and between laboratories.

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Xevo TQ-S <https://www.waters.com/10160596>

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720004400, June 2012