New Streamlined Software for Screening to Determine 250 Pesticides in Orange Oil by LC-MS/MS

Dipankar Ghosh, Jonathan R. Beck, Charles Yang, Jamie K. Humphries, Kristi Akervik, Kevin McHale

The thermo Fisher Scientific, San Jose, CA, USA

Introduction

A software program, TraceFinder (Thermo Scientific, San Jose, CA), has been developed to help researchers in the Environmental and Food Safety field. TraceFinder offers a streamlined methodology for the development of analytical methods and the analysis of the samples. The software allows researchers to choose the area they would like to begin working (Figure 1). In this poster, the entire process will be illustrated, from Method Development to Reporting. The software incorporates an LC-MS methods database that can be customized by the user to include unique compounds, in addition to preloaded methods. The method development section allows the user to choose the conditions for the chromatography, including the flow rate and the column type. The acquired data is then analyzed in the reporting section, where the results are flagged based on different criteria. For example, the user may set a flag for a compound whose calculated concentration is beyond the upper limit of linearity, above a defined reporting limit, or below a limit of detection as well as ion ratio. This allows the user to adjust the parameters to achieve the best results. The goal of this poster presentation is to demonstrate TraceFinder’s ease of use for the method development and analysis of 250 pesticides in orange oil.

Results

Method Development

The flow of TraceFinder in the Method Development section allows the user to choose the conditions for the chromatography, including the flow rate and the column type. The acquired data is then analyzed in the reporting section, where the results are flagged based on different criteria. For example, the user may set a flag for a compound whose calculated concentration is beyond the upper limit of linearity, above a defined reporting limit, or below a limit of detection as well as ion ratio. This allows the user to adjust the parameters to achieve the best results. The goal of this poster presentation is to demonstrate TraceFinder’s ease of use for the method development and analysis of 250 pesticides in orange oil.

Acquisition

The Acquisition section provides a step-by-step process to begin data acquisition. The method development is followed by the actual collection, and the final result of the screening is obtained. This allows for future batches in advance of sample preparation, for example. When the samples are run, the chromatogram is obtained and the results are displayed. The results are then analyzed in the Reporting section where the results are flagged based on different criteria. For example, the user may set a flag for a compound whose calculated concentration is beyond the upper limit of linearity, above a defined reporting limit, or below a limit of detection as well as ion ratio. This allows the user to adjust the parameters to achieve the best results.

Method

The goal of this poster presentation is to demonstrate TraceFinder’s ease of use for the method development and analysis of 250 pesticides in orange oil.

Sampling and LC-MS/MS

For all samples, the sample was spiked with a stock of 250 pesticides to give a solution containing 1 mg/mL of each pesticide. In order to receive an adequate signal, the stock solution was made up to 1 mg/mL with 50% acetonitrile and 50% water. Then, 300 µL of the stock solution was added to 3 mL of the sample. The solution was then mixed and filtered with a 0.2 µm filter. The sample was then analyzed using the Thermo Scientific Accela system and a TSQ Vantage™ EMR triple quadrupole mass spectrometer with HESI-II (Heated Electrospray Ionization) was used for the screening of 250 pesticides. The instrumental conditions were as follows:

- Ion Source Polarity: Positive and Negative ion modes
- HESI: Spray Voltage: 3500 V
- Vaporizer Temperature: 400°C
- Sheath Gas Pressure: 55 arbitrary units, Nitrogen
- Q1/Q3 Peak Resolution: 0.7 Da
- Scan Width: 0.002 Da
- Cycle Time: 0.4s

Software

Data collection and processing were handled by TraceFinder’s Environmental and Food Safety software. TraceFinder provides a user-friendly interface for the development and analysis of methods and allows for the streamlining of the process. The software generates the method for the chromatography, and the instrument is set up for the screening of 250 pesticides. The results are then analyzed in the Reporting section where the results are flagged based on different criteria. For example, the user may set a flag for a compound whose calculated concentration is beyond the upper limit of linearity, above a defined reporting limit, or below a limit of detection as well as ion ratio. This allows the user to adjust the parameters to achieve the best results.

Data Review

The logged screening analysis of 250 pesticides in orange oil was treated in the Method Development section. The software generates the method for the chromatography, and the instrument is set up for the screening of 250 pesticides. The results are then analyzed in the Reporting section where the results are flagged based on different criteria. For example, the user may set a flag for a compound whose calculated concentration is beyond the upper limit of linearity, above a defined reporting limit, or below a limit of detection as well as ion ratio. This allows the user to adjust the parameters to achieve the best results.

Conclusions

The goal of this poster presentation is to demonstrate TraceFinder’s ease of use for the method development and analysis of 250 pesticides in orange oil.