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응용 자료

Posi±ive: Improving the Workflow for TOF Pesticide Screening

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Introduction

Pesticide screening is a highly complex analysis, with differing requirements for fully-targeted MRM versus semi-targeted TOF approaches.

TOF screening has gained in popularity due to benefits, such as historical data interrogation, simplified instrumental method setup, and reduced compromise in method performance when increasing the scope of the method.

Processing and reviewing TOF pesticide screening data is often a complex workflow where positive peaks are first identified then quantified to assess the risk posed to the final consumer or environment. Frequently, the transfer from the qualitative to quantitative processes is performed manually, which places a significant drain on data review resources and introduces a high probability for errors. The typical data review stages are summarized in Figure 1, where the flow chart shows the extensively manual process that enables the question “Are any pesticides present and if yes, is that presence significant?” to be answered. Due to the time-consuming nature of this workflow, it is common to use a fully-targeted approach, where only the compounds included in calibration standards are quantified, with post processing to locate non-targeted pesticides occurring over a longer time scale. Figure 1 also displays a typical initial result report, produced using a fully-targeted approach.

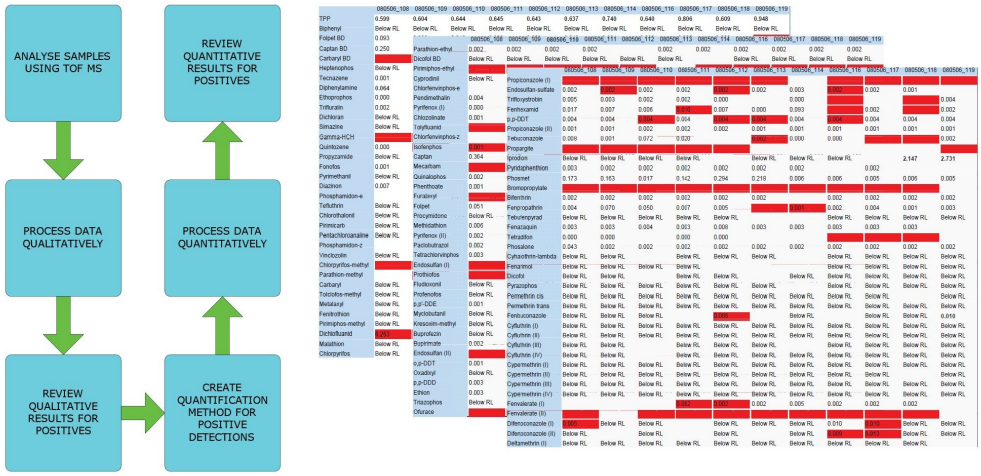

Figure 1. The traditional workflow for processing TOF pesticide screening data, with a typical initial targeted screening results summary.

Results and Discussion

Posi±ive™ enables TOF pesticide screening data to be qualitatively and quantitatively reviewed in a single pass, delivering important quantitative results for positively detected components. The flow diagram in Figure 2 shows the data processing steps involved when processing TOF pesticide screening data using Posi±ive, where all of the time-consuming data processing and review tasks are now automated. All that is needed to process data is a target compound list containing compound name, formula, and retention time. The list can be unlimited length. Data processing is fully automated, with quantified results being generated only for the positive and tentative compounds, with single mouse-click access to the qualitative results, if required.

Figure 2. The Posi±ive workflow for processing TOF pesticide screening data.

During automated processing, pos performs a qualitative search to generate presence/absence results for the compounds in the target list, using mass accuracy and retention time to determine if compounds are positively, tentatively, or negatively detected. All positive and tentative detections are then automatically quantified and displayed within a TargetLynx™ browser report. Figure 3 displays the summary result for the Posi±ive-targeted and non-targeted screening of >100 pesticides in a batch of 11 sample extracts, with the calibration curves. Using Posi±ive only the positive (exact mass and retention time within definable tolerances) and tentative(retention time OK with flagging, indicating exact mass is out of tolerance) pesticides are automatically quantified, automating the highly time-consuming results review and compound list reduction process seen in the traditional workflow, as shown in Figure 1. Thiabendazole, which is highlighted in Figure 3, is one of the non-targeted compounds(with no calibration standard)which would not have been detected using the targeted approach reported in Figure 1.

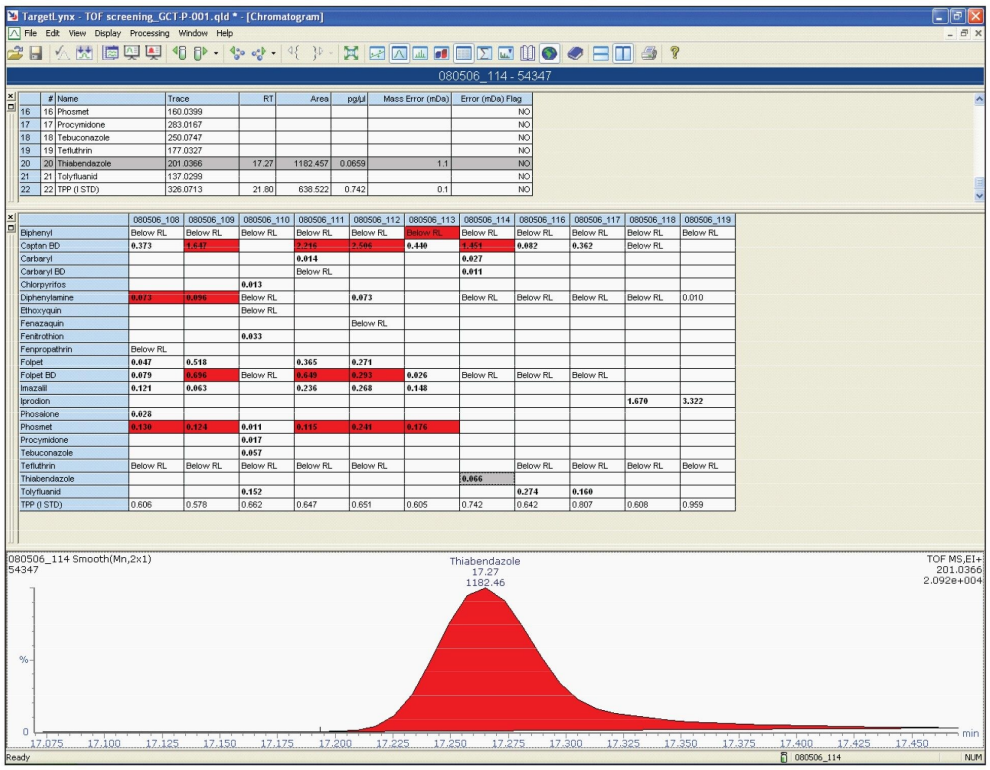

Figure 3. The Posi±ive pesticide screening results, summarizing the same batch as in Figure 1 using a targeted and non-targeted screening approach.

Conclusion

Posi±ive significantly reduces the data processing time for reviewing pesticide TOF screening data by ensuring that only the positive and tentative detections are quantified automatically.

Posi±ive reduces the manual generation of the batch-specific quantification methods from many hours to minutes.

The automated nature of processing also reduces the possibility of errors by removing manual transcription steps from the workflow.

The information-rich nature of TOF data places increasing demands upon data processing software, with

reduction in manual processing and the automation of repetitive tasks key to improving quality of results and accessibility to TOF.

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