INTRODUCTION

Chemical diversity of emerging and legacy pesticides requires the use of multiple chromatography methods for full compound coverage. Here, we propose the use of a single HRMS system equipped with an atmospheric source that can be easily switched between LC and GC sources. A suite of pesticides that are both GC and LC amenable were analyzed on a single HRMS system. Data was acquired using alternating high and low collision energy states across the full analytical mass range, such that product ions were also generated. The data was screened against a known library of compounds which was automatically interrogated using mass accuracy, isotopic fit and fragment matching. The data was also interrogated for unknown contaminants present and elucidation of the unknowns was determined with the software. The GC and LC data was handled on a single data analysis platform. Fruit and vegetable samples were spike with GC and LC amenable pesticides at regulatory reporting levels.

RESULTS

Figure 1. Qualitative and quantitative workflow for pesticides screening analysis.

Figure 2. HRMS data for identifications in non-spiked (blank) green bean QuEChERS extract found using UPLC and APGC injections.

Figure 3. Halogen match is used for identifying unassigned spectral peaks which have a $-\text{Cl}$ or $-\text{Br}$ isotope distribution pattern. Following spectral and chromatographic display (A), database searching and fragment matching is performed for confirmation of structure (B).

CONCLUSIONS

- Universal atmospheric pressure source design afforded full compound coverage through the use of both LC and GC inlets on a single HRMS platform
- Full spectral acquisition of both low and high energy data provided accurate mass precursor and product ion information for confident detection and determination of non-targeted components
- Streamlined acquisition and processing software was utilized to deconvolute and review both data sets in a streamlined and efficient workflow approach
- Apex peak picking allows data files to be transformed to component tables. These component tables can be interrogated for targeted, suspect and unknown compounds of interest—WITHOUT the need to reprocess data.