Benefits of Chemical Ionization in GC-MS/MS Analysis using the Xevo TQ-GC

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

Abstract

To test the performance and robustness of Xevo™ TQ-GC's CI source in GC-MS/MS analysis.

Benefits

The Xevo TQ-GC provides rapid, tool-free changeover between EI and CI.

Introduction

In traditional GC-MS/MS analysis, the technique that is most often utilized is electron ionization (EI). However in some cases, compounds can be labile and fragment heavily when using EI, which can make it difficult to identify them via NIST library searches, or to generate selective MRMs. Chemical ionization (CI) operated in both positive and negative ion modes can help reduce the fragmentation significantly. By utilizing the dedicated CI ionization source available on Waters™ Xevo TQ-GC, which was designed for extended robustness and rapid tool-free changeover, both EI and CI experiments can be performed on the same system.

Figure 1. The Xevo TQ-GC is designed for simple, tool-free changeover between Electron ionization (EI) and Chemical ionization (CI) in less than 10 minutes.

Results and Discussion

In order to perform CI experiments on the Xevo TQ-GC, the inner ionization source must be changed. Switching between EI and CI on the Xevo TQ-GC is very simple and does not require tools. Changing between EI and CI takes less than 10 minutes, with additional time required to pump down the instrument after the changeover. In CI ions are produced via collisions with the reagent gas (e.g. methane, ammonia, or isobutane). In the experiments described here, methane was used as the reagent gas. Inside the ion source, the reagent gas is present in large excess relative to the analyte. Electrons entering the source will preferentially ionize the reagent gas. The molecules then collide with the reagent gas ions to produce ions.

In order to demonstrate the chemical ionization capabilities of the Xevo TQ-GC, replicate injections were performed in CI+ and CI- modes. In the first experiment 15 injections of a grape extract spiked at 0.1 mg/kg

containing five pesticides were run in CI+ mode (Figure 2). In the second experiment, the same extract was run 15 times to analyze an additional five pesticides in CI- mode (Figure 3). The reproducibility for the CI experiments was excellent, and the response maintained was consistent throughout the run with %RSDs <10%.
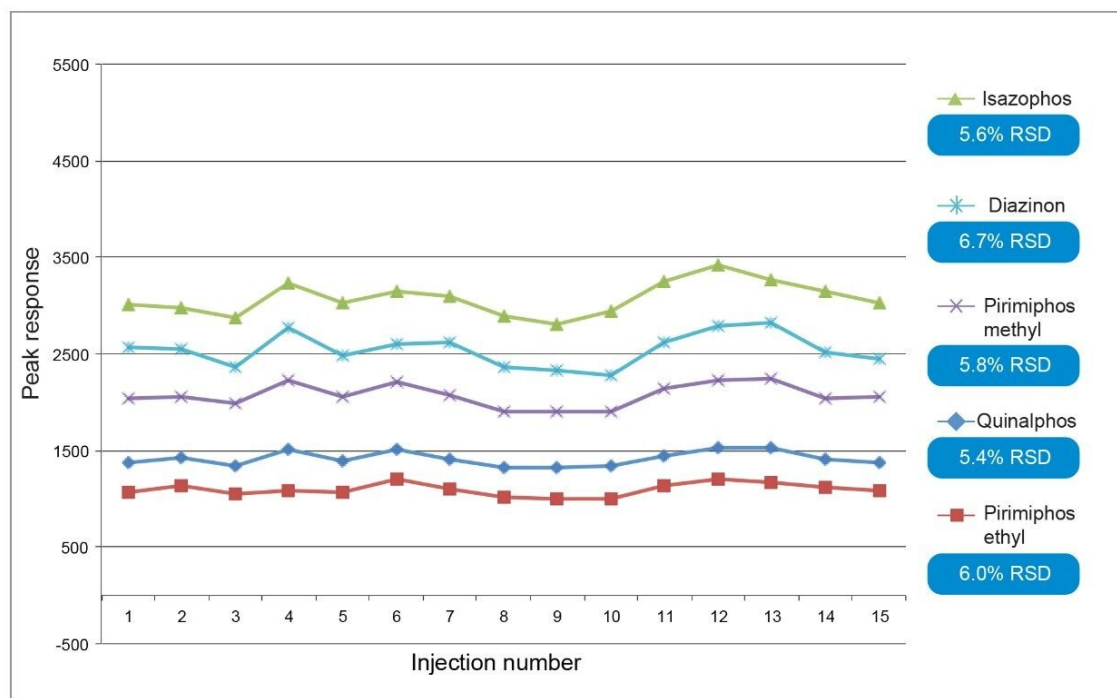

Figure 2. Repeatability from replicate (n=15) injections of grape extract containing five pesticides at 0.1 mg/kg in CI+.
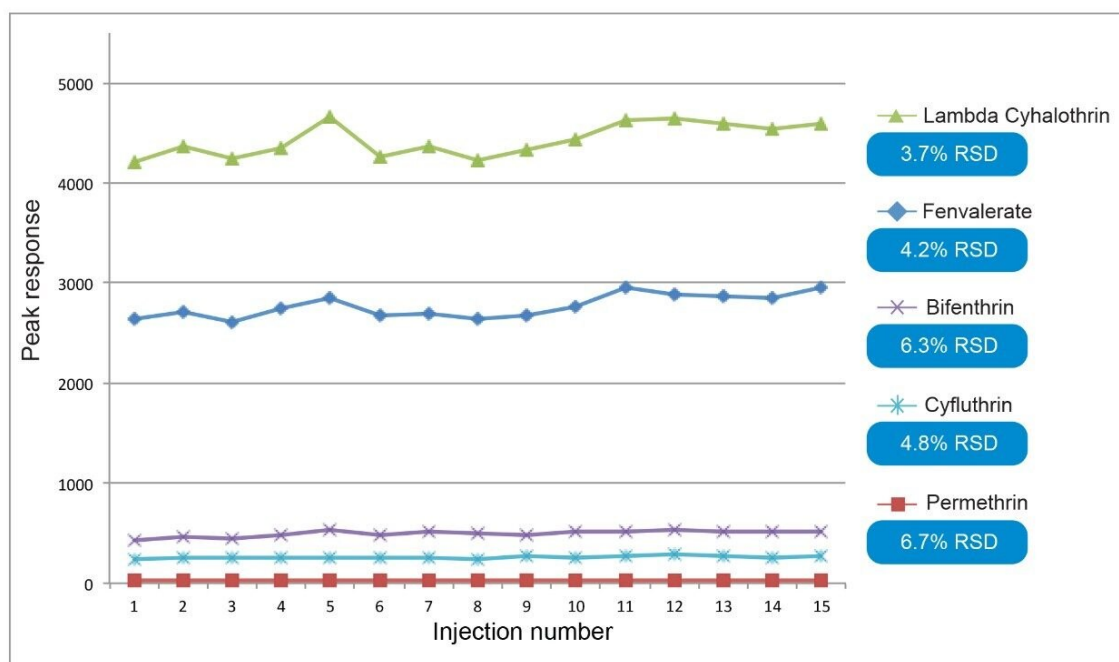
Figure 3. Repeatability from replicate (n=15) injections of grape extract containing five pesticides at 0.1 mg/kg in CI-.

Conclusion

The Xevo TQ-GC has been shown to produce consistent results in CI mode by utilizing the dedicated CI source. The changeover between EI and CI modes is easy to perform and requires no tools. The Xevo TQ-GC showed excellent reproducibility in both CI- and CI+ modes.

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