Nota applicativa

Demonstration of Collision Cross Section (CCS) Value Conservation Across LC and GC Analyses

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

Abstract

This application brief demonstrates the conservation of CCS values for 73 pesticides introduced under both GC and LC conditions.

Benefits

CCS values are robust and precise values associated with physical properties of an ion, and are conserved regardless of chromatographic technique implemented.

Introduction

Contaminant identification in food and environmental matrices using both GC and LC-MS techniques are widely implemented, although challenges with matrix effects, false detections, and reproducibility of ion ratios exist. In this technology brief we demonstrate the application of travelling wave ion mobility spectrometry (TW-IMS) coupled to a quadrupole time-of-flight (QTof) MS to generate a robust and unique additional identification point for contaminant analysis. The determination of a collision cross section (CCS) of an ion can be extrapolated from the observed drift time as the ion passes through the drift cell. To demonstrate the robust and precise nature of CCS values, a suite of pesticides were analyzed under both GC and LC conditions, and the CCS values obtained compared.

Results and Discussion

A comparison of 73 GC and LC amenable pesticides that had been injected as solvent standards five times each during both the LC and GC analyses found CCS values that were strongly correlated to one another (Figure 1).

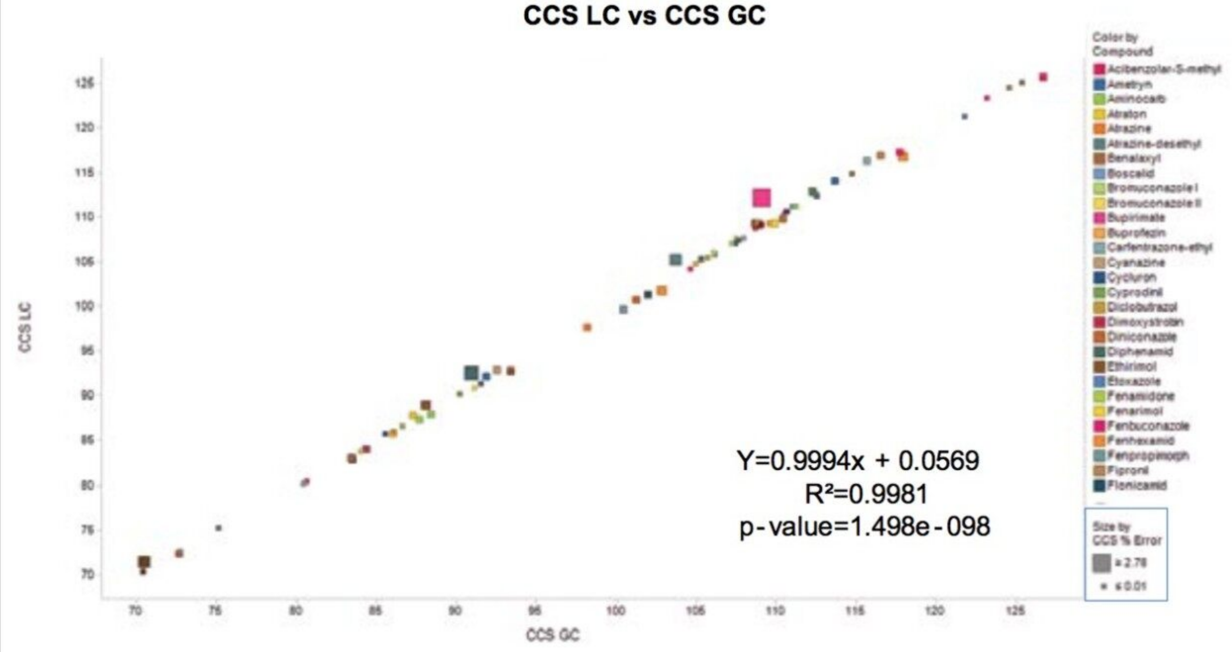

Figure 1. CCS value regression analysis of GC and LC analyses, indicating conversely to the RT comparisons, a strong correlation between CCS measurements obtained under GC and LC analyses for the 73 pesticides.

A regression analysis of the LC and GC results for CCS produced an R^2 value of 0.998, indicating a very high degree of correlation. Moreover, the CCS values across the five injections in each technique showed minimal deviation.

When retention times under the two techniques were compared, as would be expected, no correlation was observed (Figure 2). From these results, it could be seen that CCS values represented a unique property of the ions generated that was well conserved, regardless of that analytes introduction into the travelling wave ion mobility MS system. These results support the use of CCS values, in addition to mass and characteristic product ions, for compound identification.

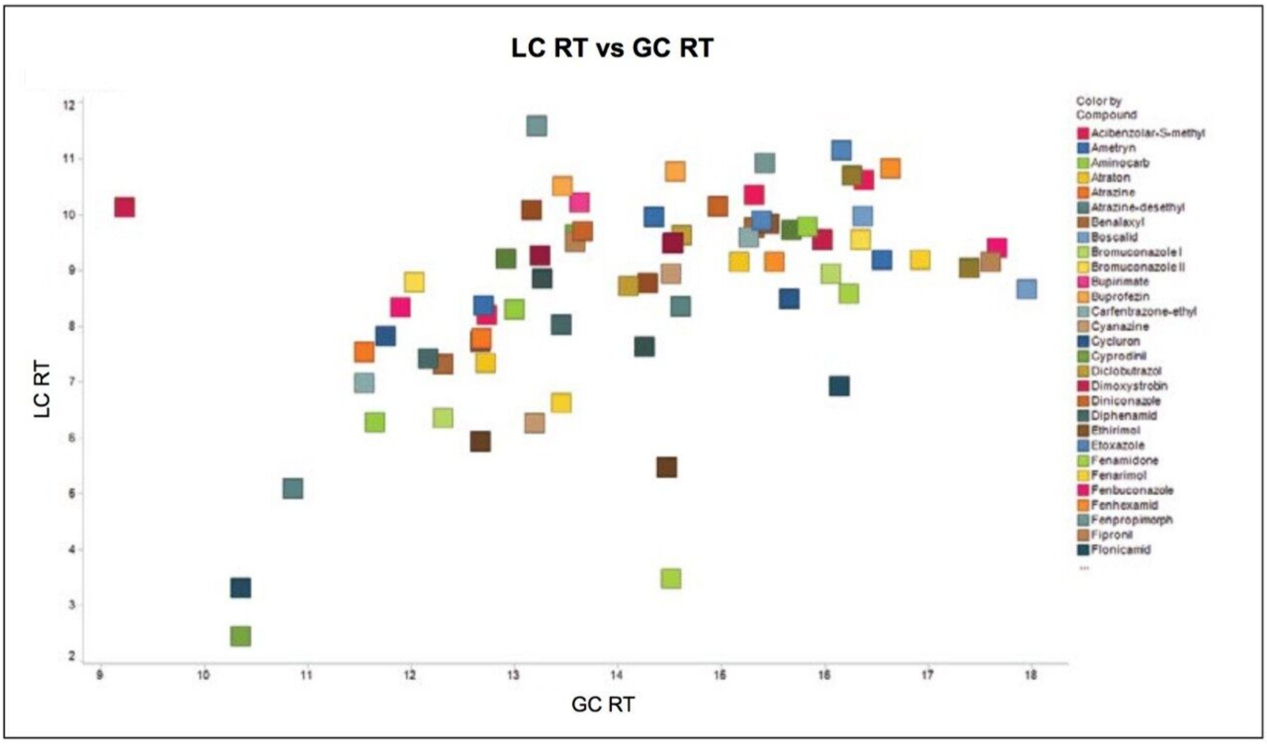

Figure 2. Retention time regression analysis of GC and LC analyses, indicating no correlation between the two approaches for 73 pesticides analyzed.

Conclusion

CCS values are unique properties of an ion in the gas phase that are retained regardless of the method used to introduce the analytes into the MS system. Using CCS values in contaminant screening offers a unique point of identification, and allows flexibility around retention time tolerances applied for identification purposes.

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