Waters™

アプリケーションノート

Identifying Analytes Using NIST Library Searching of Xevo TQ-GC System Data

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

Abstract

To demonstrate the ability of the Xevo™ TQ-GC System to generate EI spectra that match the corresponding spectra in the NIST Standard Reference Database v17.

Benefits

Identification of unknowns through library searching of EI data.

Introduction

EI GC-MS is a well established technique for the analysis of unknowns. One property of EI in particular, the ability to generate rich, characteristic fragmentation patterns reproducibly, is important to the success in using EI data to identify unknown compounds. Because EI fragmentation is a well characterized technique, it is possible to interpret an EI spectrum to determine the elemental composition of an unknown. However, this process is extremely time consuming and not amenable to automation. For these reasons library searching of EI spectra against a database of thoroughly curated reference spectra is the most common technique

employed to identify analytes in a GC-MS analysis.

Results and Discussion

The Xevo TQ-GC System was operated in full scan EI mode for analysis of GC-MS samples containing pesticides. It is worth noting that while this instrument is a tandem quadrupole it is also able to perform all of the same experiments that a single quadrupole GC-MS system would be used for such as full scan, SIR and combined scanning plus SIR. In Figure 1, the upper spectrum is the experimental data and the lower spectrum is from the NIST library. The reported probability of 96.2% is a good initial indicator of a high-quality match between the two spectra. The graph in the upper left indicates good differentiation of the spectrum for this compound from other possibilities returned by this search. And, a final visual comparison between the two spectra shows good correspondence through evaluation of the presence or absence of characteristic peaks, as well as the relative abundance of spectra peaks.

Because chloroneb is a relatively low molecular weight (206) and early eluting (retention time index [RTI]1508), a second high mass, later eluting compound was also selected for evaluating the library search quality of the data. The results for mirex, molecular weight 540 and RTI 2530, are shown in Figure 2. As with the earlier example, there is a high probability of 97.3%, good differentiation from other search results indicated by the graph and good correspondence between the acquired and reference spectra.

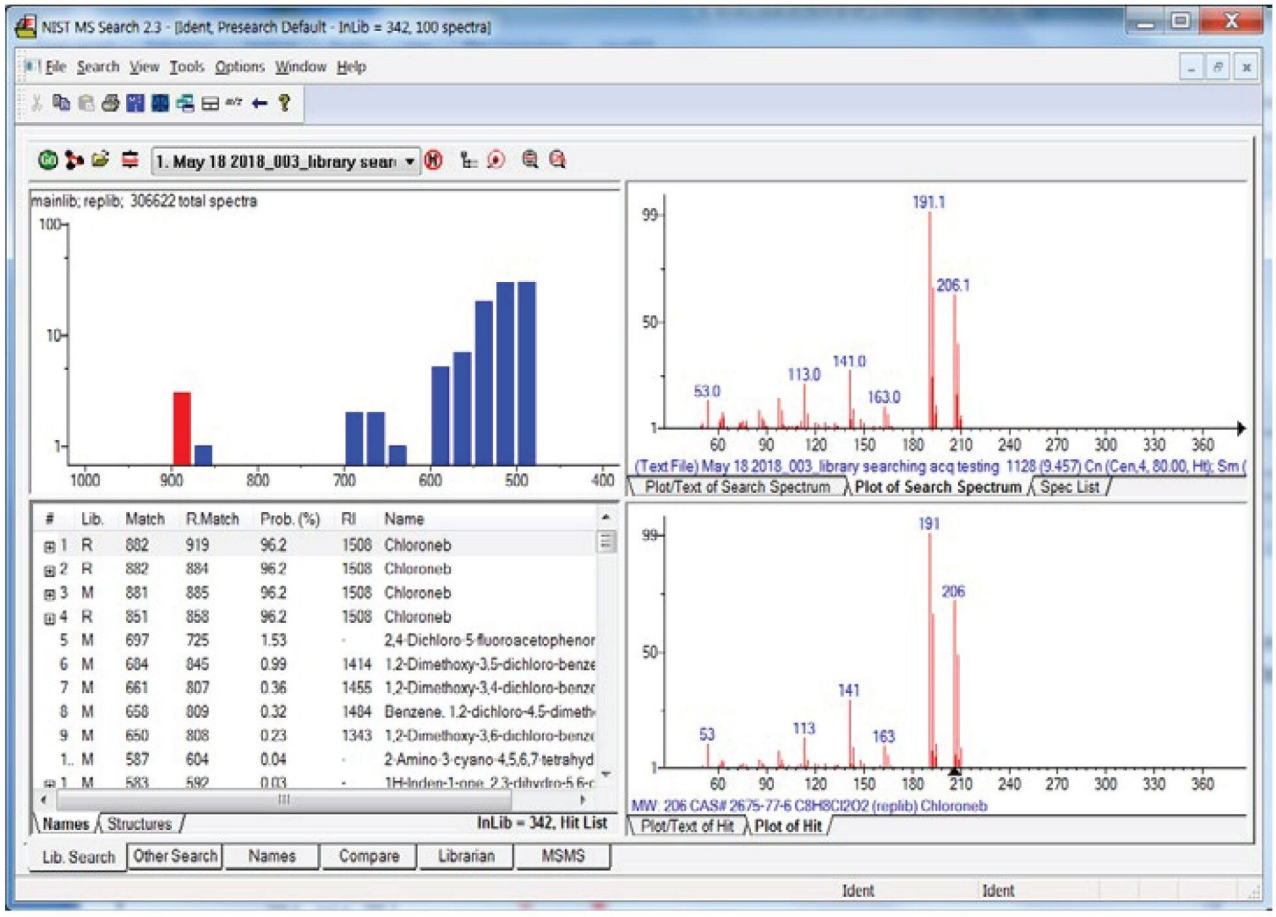

Figure 1. NIST library search results for chloroneb.

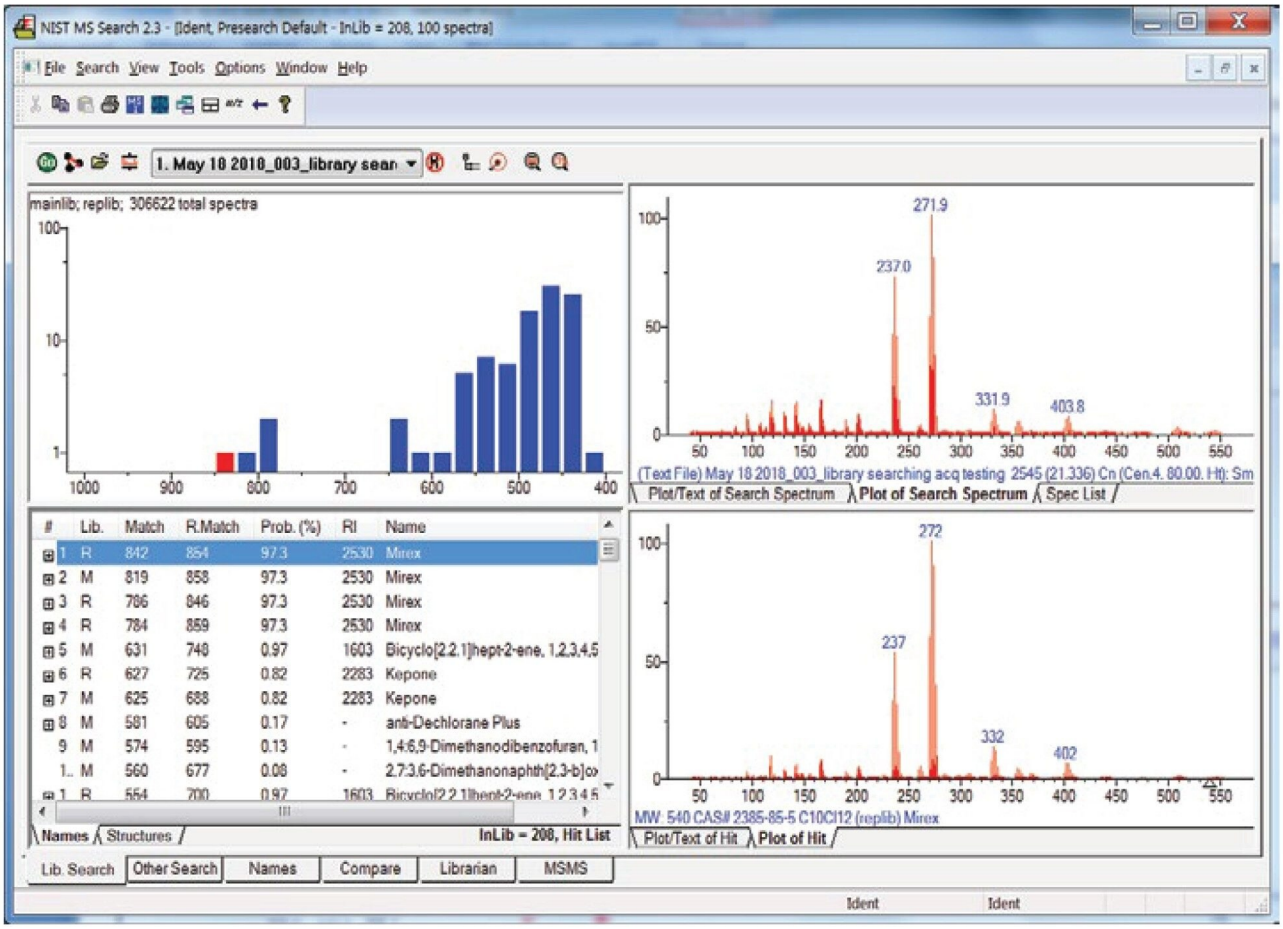

Figure 2. NIST library search results for mirex.

Conclusion

The ability to use automated library searching to identify unknowns in a GC-MS analysis is a common need in many labs. EI data from full scan experiments on the Xevo TQ-GC demonstrates the ability of this system to successfully identify pesticides using a NIST library search. The full scan data can be acquired concurrently with MRM data on the Xevo TQ-GC using RADAR which brings NIST searchable spectra to targeted analysis.

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Xevo TQ-GC Mass Spectrometry System <https://www.waters.com/waters/nav.htm?cid=134977323>

RADAR <https://www.waters.com/134798882>

720006365, August 2018