AMDIS – Automatic Mass Spectral Deconvolution and Identification Software

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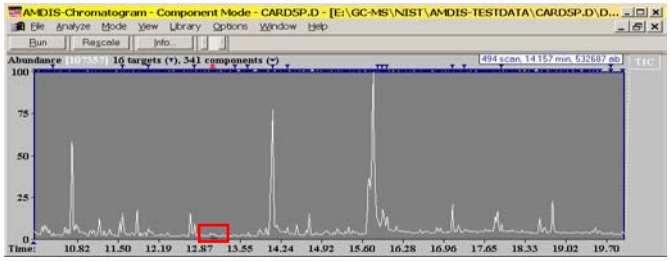
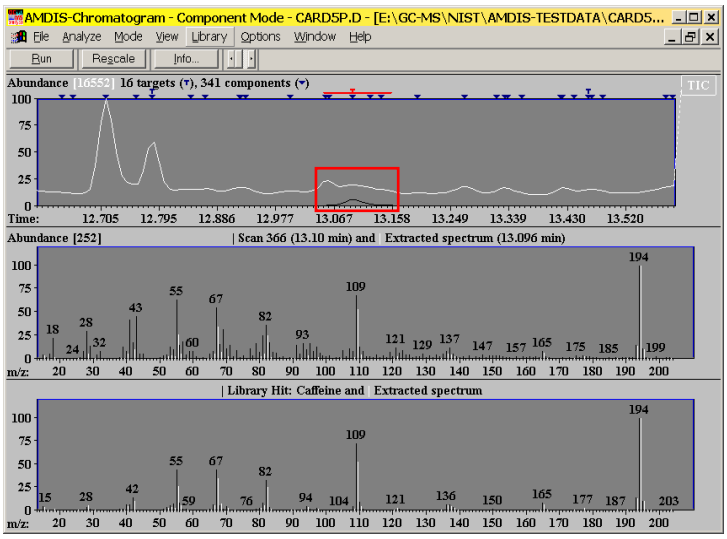
One of the most powerful tools for the analysis of complex mixtures is the combination of the gas chromatograph (GC) to separate the mixture into component parts, followed by the mass spectrometer (MS) to identify each component as it is eluted. This combination GC/MS is the most widely used analytical tool for low-concentration analysis for food safety and environmental monitoring. In addition it is widely used in general organic analysis, the development of new flavoring agents, the analysis of fragrances, and in many medical applications.

At extremely low concentrations, it can be difficult to extract the signal from the data file due to the very complex background that is present. The time spent by an analyst trying to analyze the data file can be many hours. AMDIS is a solution to this problem.



NIST's Automatic Mass Spectral Deconvolution and Identification Software (AMDIS) was originally developed for detection of chemical weapons in complex mixtures such as might be found in the environment or in chemical process streams. It was designed to work without analyst input as a method of insuring that sensitive business information that could be present in a process stream was not compromised.



The data that AMDIS analyzes, such as those shown above (which is a plot of total MS ion current as a function of elution time from a GC) are not typically the large obvious peaks, rather they are the very small components that are not obvious to the user. In this case, AMDIS extracted 341 distinct components from this data file (information provided by the components label in the figure). Typical software provided with the instruments might have found 50, and the analyst would have still had more work to do to identify the large majority of peaks. AMDIS can of course analyze the larger peaks, but the time spent by the analyst on these is small and in most cases the answer is known before the analysis is done. It is the small components that can change the flavor, can be the toxic residues, and can be the indicator of disease. It is in extracting these small components that AMDIS excels. Shown in the figure to the right (in the top window) is an enlargement of the region indicated by the red rectangle in the previous figure. This is the location of the caffeine found in the data file. In the second window is a mass spectrum from the region (in red box the elution time plot) where the caffeine was found. The signal in this region is very small, as indicated by the full-scale abundance in each window. Here the white lines (displayed next to the extracted peaks) indicate the portion of the data that was used for identification the caffeine. The bottom panel shows the extracted data (again in white) compared to the library spectrum of the caffeine. The entire process takes a few minutes rather than the hours that an analyst would take to do determination manually.

In the above example (cardamom oil with very low levels of pesticides) AMDIS found the pesticides, but also found low levels of caffeine.

Agilent Technologies incorporated AMDIS into a new set of tools for automatic analysis under the general name of Deconvolution Reporting Software.

In the last year the growth in the use of AMDIS by the organic analytical community has been very strong. One of the most exciting developments has been the incorporation of AMDIS into a new set of tools for automatic analysis developed by Agilent Technologies. The tools have been given the general name of Deconvolution Reporting Software (DRS) and incorporate Agilent Technologies run time locking technology, the NIST search software, and AMDIS in a combined tool. DRS allows users to identify pesticides more confidently and at lower concentrations and with more confidence than had been possible with the Agilent system alone.