Automated Gas Chromatograph-Mass Spectrometer Analysis

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Introduction

GC-MS data are information rich. Analysis can be time consuming, especially when examining complex analytes. We present a new computer system that combines fast, flexible automated deconvolution, with automatic database search to identify knowns and unknowns. Novel compounds can be identified, and structural characteristics deduced by applying MS Adaptive search that uses fragmentation and structural data to propose likely structural details of the unknown.

Method

Our system follows individual m/z values across multiple spectra and extracts a pure spectrum from the data for each individual component while trying to separate components with overlapping m/z value peaks. If accurate m/z value data are available and the user selects to use it instead of unit m/z values, the chosen instrument accuracy (automatic, ppm, or fixed value) is used to determine the correct accurate m/z values that exist in the entire GC-MS analysis. The m/z values in the raw data are converted into correct accurate values based on the closest value found taking the instrument resolution into account. The corrected m/z values form the basis of the following deconvolution.

During the deconvolution step, individual m/z values are pursued across multiple raw spectra, and a component spectrum is extracted from the data for each individual component while trying to separate components with overlapping m/z value peaks. The details of the algorithm are summarized to a large extent by the following papers1-4.



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Method continued

Additional steps are added to automatically detect components with low intensity reconstructed total Ion Current (RTIC) chromatographic peaks, as long as they can be well-separated from neighboring components.

Results

Figure 1 shows the deconvoluted GC-MS data of nominal resolution where ion m/z values are integers, along with the database search results for each component. In our software, component Hit List parameters can be adjusted. The RTIC chromatogram pane can be selected to include the range bar to add peaks manually, then the calculations are re-run automatically to perform a new analysis.



Figure 1. A - Deconvoluted GC peak with found matches from reference MS databases; B - selected ions in a component; C - reference ion(s) used to model a component; D – extracted spectrum (top) vs. reference spectrum (bottom); E - components

Results continued

table; F- combined spectrum search and reverse search Hit Quality Index (HQI).

For accurate *m/z* value data, without knowing the instrument resolving power, there is no safe algorithm to automatically calculate this value. Therefore, we use what our research considers a reasonable value by default that has a constant component and a variable component depending on mass (ppm). Empirically, this works in most cases. Increasing the *m/z* value accuracy too much incurs the danger of splitting an induvial *m/z* value into individual mass spectral peaks that should be considered as just one. Decreasing the *m/z* value accuracy too much may cause individual mass spectral peaks to be merged resulting incorrect accurate *m/z* values to be reported.

If a user knows the instrument's resolving power, that value should be entered in the highlighted dialog in figure 2 and possibly be saved into a profile.



Figure 2. One can use highlighted "Input Data Resolution" to set the resolution for the data file.

Also, as seen in Figure 2 component Hit Lists are easily reported.

This new user-friendly application is user friendly, coupled with reference MS spectra, can greatly improve the efficiency of time-consuming GC-MS data analysis.



Summary

References

- 1. S. E. Stein. An Integrated Method for Spectrum Extraction and Compound Identification from Gas Chromatography/Mass Spectrometry Data. JAm Soc Mass Spectrom 1999, **10**, 770 –781.
- **2.** R. G. Dromey, Mark J. Stefik, Thomas C. Rindfleisch, Alan M. Duffield. Extraction of Mass Spectra Free of Background and Neighboring Component Contributions from Gas Chromatography IMass Spectrometry Data. ANALYTICAL CHEMISTRY, 1976, VOL. 48, NO.9, 1368-1375.
- **3.** J. E. Biller, K. Biemann. Reconstructed Mass Spectra, A Novel Approach For The Utilization Of Gas Chromatography-Mass Spectrometer Data. Analytical Letters 1974, 7, 515-28.
- **4.** Bruce N. Colby. Spectral Deconvolution for Overlapping GC/MS Components. J Am sot Mass *Spectrom* 1992, **3**, 558-562.