Agilent Technologies
Innovating the HP Way

Automated Mass Spectrometry Deconvolution and Identification System

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Technical Note

A New Dimension in Analyzing GC/MSD and LC/MSD Data

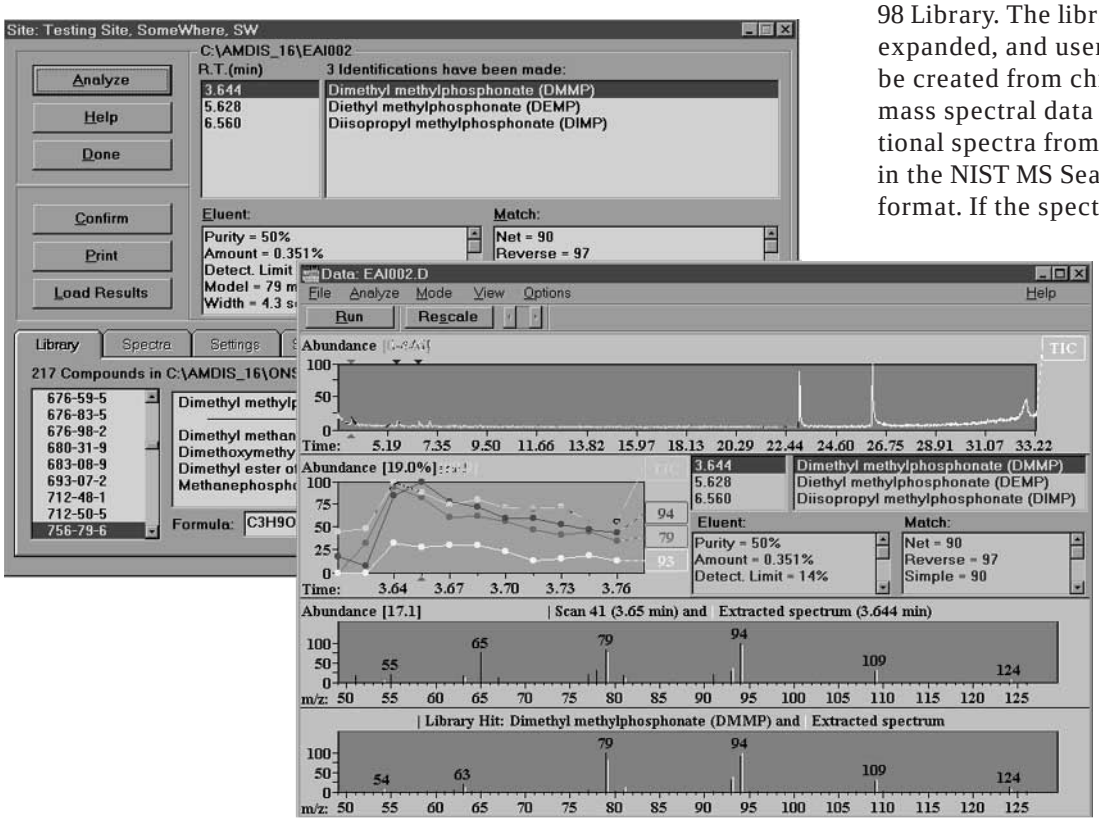
Agilent Technologies ChemStation

Overview

The Automated Mass Spectrometry Deconvolution and Identification System (AMDIS) deconvolutes impure GC/MSD and LC/MSD mass spectra (which can result from coelutions or background contaminants) and displays the reconstructed chromatograms. The reconstructed chromatograms can be further processed to distinguish pure spectra from the spectra of mixed substances. The pure spectra can then be analyzed against libraries of target compounds or against the NIST 98 Library (the 1998 edition of the NIST/EPA/NIH Mass Spectral Library).

Pure Spectra from Mixtures

The AMDIS program uses mass spectral information to extract pure spectra from data obtained from substance mixtures by GC/MS or LC/MS. Whether working with electron ionization (EI) GC/MS data or with in-source collision-induced dissociation (CID) LC/MS data, positive determination of the presence or absence of an analyte can be made using special libraries. AMDIS is provided with individual target libraries of EI spectra for use in four applications: environmental, drugs-of-abuse, toxicological, and flavor/fragrance. All of these target libraries are derived from the NIST 98 Library. The libraries can be expanded, and user libraries can be created from chromatographic/mass spectral data or from additional spectra from other libraries in the NIST MS Search Program format. If the spectrum is not



that of a compound in one of these special libraries, it can be searched against the entire NIST 98 Library by using the NIST Mass Spectral Search Program for Windows[a]. If this search still does not reveal a good candidate for the identity of the unknown, the NIST MS Search Program's Substructure Identification routine can be used to provide a better identification.

Mass Spectra Plus Retention-Time Information

To further ensure positive identification and to reduce the risk of false-positive identifications, internal standards can be used to establish retention-time data. Custom mass spectral and retention-time libraries can be built from the identified spectra and then used for future comparisons with similar samples. Customized mass spectral libraries can also be built from the NIST 98 Library by selecting and saving the desired spectra. When ChemStation software is used and when user-created mass spectral libraries exist, they can be easily copied into NIST MS Search Program libraries. The newly created NIST Library formats are then used to produce AMDIS libraries.

AMDIS can also be used to analyze mass spectral data files without the use of user-contributed libraries. In this mode of operation, deconvoluted spectra are generated that can be interpreted or searched for using the NIST MS Search Program. Deconvoluted spectra are presented overlaid on the raw data along with overlaid and color-separated mass chromatograms of significant ions resulting from the deconvolution.

The search for AMDIS deconvoluted spectra is limited to the NIST/EPA/NIH Mass Spectral Database using the NIST Mass Spectral Search Program for Windows. The deconvoluted spectra cannot be searched against the NIST/EPA/NIH Mass Spectral Library by using the proprietary search software provided in the GC/MSD or LC/MSD ChemStation software.

The Origin of AMDIS

Biller and Biemann (1) introduced chromatographic peak deconvolution from mass spectral data in the 1970s using a maximizing-mass algorithm they had developed. The algorithm was further enhanced by Colby (2) in the early part of this decade. Since then, component identification of simple and complex mixtures in GC/MS and LC/MS data has been brought to near- perfection.

AMDIS was developed at the National Institute of Standards and Technology (United States Department of Commerce) with the support of the Defense Special Weapons Agency (DOD) for verifying compliance with the major international chemical warfare nonproliferation treaty (Chemical Weapons Convention) just signed into law by the United States Government. To make sure AMDIS lives up to its claim of no false-positive identifications, the program has been tested on over 30,000 data files against a library of potential Chemical Warfare agents.

To Obtain AMDIS

The AMDIS program is distributed only with the NIST 98 Library and the NIST Mass Spectral Search Program. The ChemStation versions of the NIST 98 Library and the NIST Mass Spectral Search Program are available as products G1033A NIST MS Library bundle and G1043A NIST MS Library upgrade, respectively. The G1041A Upgrade will be available in June 1998. Consult your local sales representative for more information.

References

1. Biller, J. W.; and Biemann, K.: Reconstructed Mass Spectra. A Novel Approach for the Utilization of Gas Chromatographic Data. *Anal. Lett.*, *vol. 7*, **1974,** pp. 515–528.

2. Colby, B. N.: Spectral Deconvolution of Overlapping GC/MS Components. *J. Am. Soc. Mass Spectrom.*, *vol. 3(5)*, **1992,** pp. 558–562.

**Printed in the U.S.A. December 1999
(23) 5967-5735E**