GC/MSD Libraries for the MSD ChemStation

Technical Note

MSD ChemStation

Routine identification of organic compounds usually requires that the mass spectra of the unknown compounds in a sample be compared with published spectra. Two main types of spectra libraries are available, the general-purpose ones (Wiley and NIST) and the specialized ones (Stan and Pfleger). In response to the need for broad-based compound identification, the Agilent MSD general-purpose libraries offer large numbers of the spectra of many kinds of molecules. If nothing is known about a compound, these general-purpose libraries would be the ones to use in a first-pass search. If the class of a chemical is known, then specific mass spectral libraries (e.g., pesticide/drug) of special compound classes can search faster, but they are only available for selected classes of compounds.

General-Purpose Libraries

The Wiley (*http://www.palisade.com*) and the National Institute of Standards and Technology (NIST: *http://www.nist.gov*) MS libraries contain 390,000 and 129,000 spectra, respectively. Some compounds in these libraries are characterized by more than one mass spectrum. Because the multiple spectra of a given compound will have been acquired under different experimental conditions these spectra may be slightly different. NIST has recently completed a 10-year review of its 107,000-compound library using the Agilent MSD. That review led to thousands of deletions from and modifications to the older 74,000-compound library. This ongoing spectral reviewing process results in better match probability and, consequently, in higher-confidence compound identification.

Agilent Technologies
Innovating the HP Way

The default library search and spectral evaluation of mass spectra in the Agilent MSD Productivity ChemStation uses the Probability Based Matching algorithm developed by F. McLafferty. This algorithm compares the spectra of unknown compounds with spectra in libraries by comparing statistically significant ions. The abundance is also evaluated, and unwanted spectra are eliminated before the search. This speeds up the search process and increases the accuracy of its results (see Figure 1).

As an option, one can use the NIST database of Chemical Structures (Part No.G1036A) to visualize the compound. The CAS (Chemical Abstracts Number) is the link between the library search results and the structures database. Using the CAS number, users can add their own structures to the database. The structures can be incorporated with mass spectra to create a more informative report. The structures can be used with any library (user-created libraries included) utilizing the CAS to link the structural database to the user-created library.

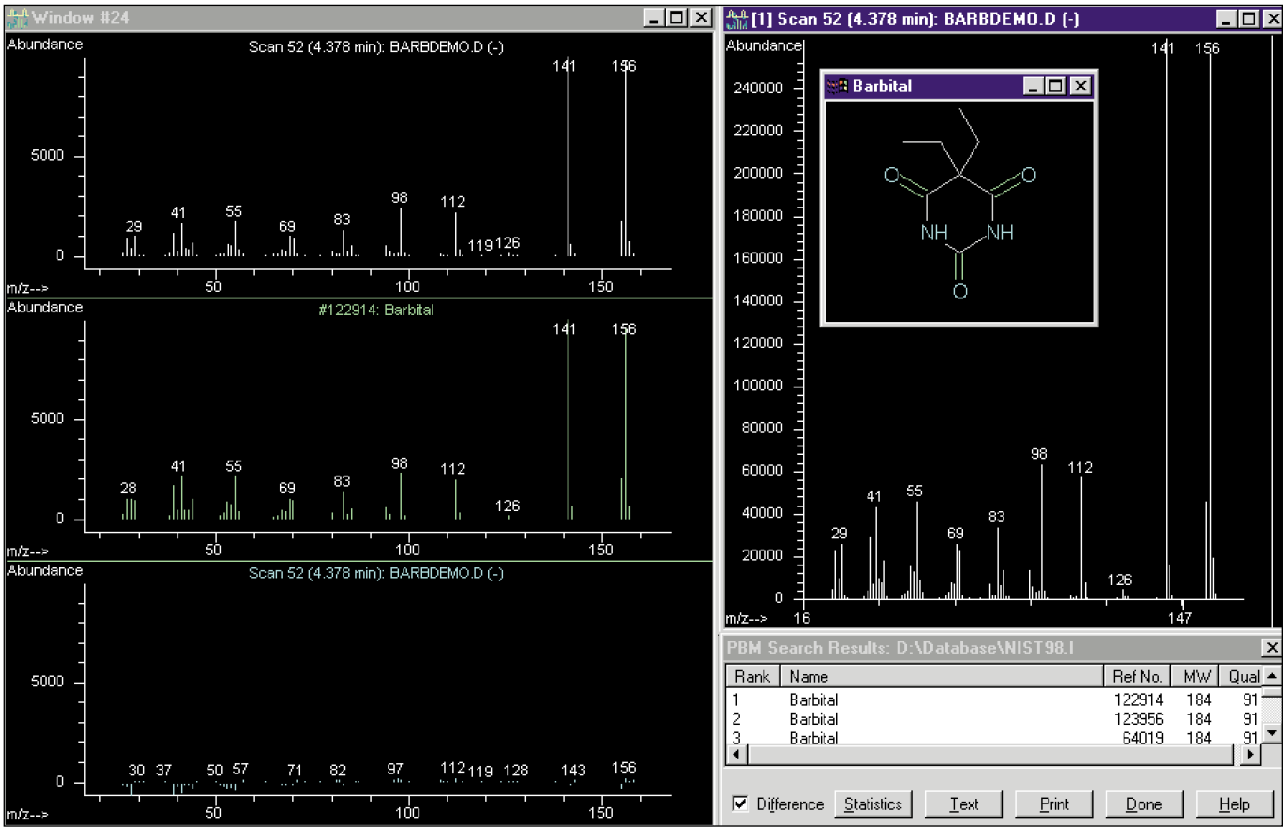

Figure 1. Example of a library search results using the Agilent MSD ChemStation software.

MSD General-Purpose Libraries

The NIST 98 Library (Agilent Part No. G1033A): National Institute of Standards and Technology.

The NIST 98 Library contains 107,886 compounds with spectra; 21,250 replicate spectra; 107,829 chemical structures; and 13,205 compounds with replicate spectra.

The Library also includes the following additional utilities:

1. the NIST Forward Library Searching Program (version 1.7);
2. the Automated Mass Spectral Deconvolution and Identification System (AMDIS) (version 2.0); and
3. the MS Interpreter (Structural/Spectrum Analysis Tool).

Wiley 7N Edition (Agilent Part No. G1035B): Wiley Registry of Mass Spectral Data, 7th Edition.

The Wiley 390K Library contains 316,934 unique compounds; 621,660 chemical names. In addition, the Wiley 7N includes a large percentage of the NIST98 library.

MSD Application-Specific Libraries

Stan pesticides (Agilent part No. G1038A):
The Stan Library, H. J. Stan, Technische Universitaet Berlin).

Pfleger drugs and metabolites (Agilent part No. G1039C):
Pfleger, Mauler, Weber (A. Pfleger, Universitaet Homburg-am-Saar)

Mass Spectra Libraries: Summary

Information about the two general-purpose and two application-specific spectra libraries is summarized in the following table.

Library name	Part number	Number of spectra	Number of compounds
NIST 98 Bundle *	G1033A	129,136	107,886
NIST Structures	G1036A	N/A	107,829
Wiley 7N edition	G1035B	390,000	316,934
Stan Pesticide	G1038A	340	340
PMW 3rd edition	G1039C	6,300	6,300
Upgrades			
NIST98	G1041A		
Wiley	G1730A		
PMW	G1731A		

* NIST98 Bundle includes the NIST98 Search Program, the NIST98 Format Library, the NIST98 PBM Format Library, and the NIST98 Structures.

For more information on our products and services, you can visit our site on the World Wide Web at: **http://www.agilent.com/chem**.

Printed in the USA October 2000
Rev. 1
(23) 5967-5807E

Agilent Technologies
Innovating the HP Way