

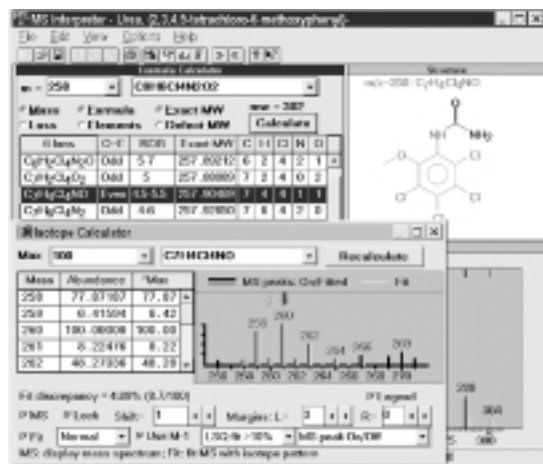


## Adding User-Drawn Structures

Users may import their own chemical structures with selected user spectra. This is done in the Tools/Librarian section of the program by connecting a user-drawn structure in standard MOL-file format with a user spectrum. As before, if a user spectrum is given its CAS registry number and the Main Library has a structure for it, this structure will automatically be shown with user spectra unless the user has attached an imported structure to the spectrum.

## Aids for Automation and Reporting

A variety of methods for automated searching and reporting of results are available. From the File menu selection, if Print automation is on, printing will follow each library search. A set of print options is also available from the "User Search Options" Window (select Search, then User spectrum). This is of particular use when using this NIST Program with other data acquisition programs.

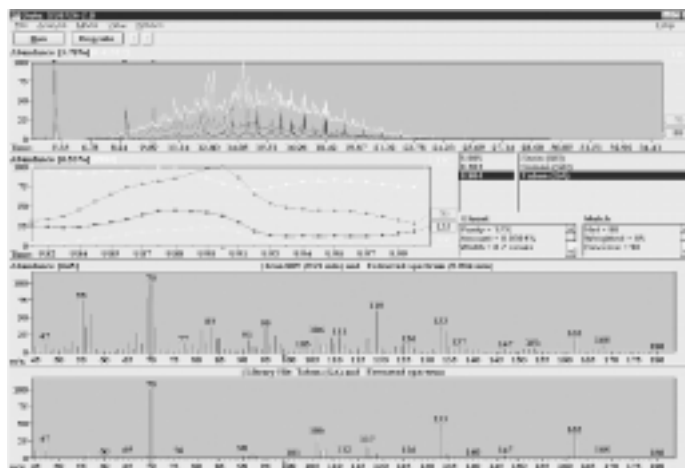


## Automated Mass Spectrometry Deconvolution and Identification System (AMIDIS)

Extract pure component spectra from complex GC/MS or LC/MS data files and search against specialized libraries or the NIST library. This module was developed at the National Institute of Standards and Technology (NIST) for the critical task of verifying a major international treaty, the Chemical

Weapons Convention. After two years of development and extensive testing it is now being made available to the general analytical chemistry community. Identification can be aided by internal standards and retention times. Libraries can be built directly from analyzed data files or from spectra in the NIST/EPS/NIH Database. AMDIS can also serve as a preprocessing tool for the GC/MS data files, automatically performing noise reduction for all components. It permits traditional library searching for any selected component. A flexible interface is provided to assist the analysis of complex matrices.

Included as a separate utility, AMDIS attempts to reconstruct original mass spectra for individual components in arbitrarily complex GC/MS and LC/MS reconstructed total ion current (RTIC) chromatograms; and, if a target library is provided, can directly identify target compounds. AMDIS is especially useful when an RTIC chromatographic peak represents multiple components. Regardless of each component's concentration, pure mass spectra are deconvoluted for analyses. AMDIS was developed by NIST in order to meet the rigorous requirements of the Chemical Weapons Convention. AMDIS was tested against more than 30,000 GC/MS data files accumulated by the EPA Contract Laboratory Program without a single false-positive for the target set of known chemical warfare agents. While this level of reliability may not be required for all laboratories, this shows the degree to which the algorithms have been tested.



Part No.	Description	Price
541010	NIST 05 Library & Search Program, Standard version for most MS data systems.	
541010UG	NIST 05 Upgrade from NIST 98/02*	
541010HP	NIST 05 Library & Search Program for Agilent ChemStation*	
541010HPUG	NIST 05 Upgrade for Agilent ChemStation*	

+ - Standard version includes NIST database in native NIST format. NIST MS search software integrates directly with many MS data systems, or you can import spectra to be searched through AMDIS.

\* - Chemstation version is identical to standard version but also includes NIST database in Chemstation (.L) library format for direct integration with Chemstation PBM library searching