

NIST 98

*A Major New Release available from
Scientific Instrument Services*

NIST/EPA/NIH Mass Spectral Library

*The product of a multiyear, comprehensive evaluation and expansion of the
world's most widely used mass spectral reference library*

Evaluated for Quality

each spectrum critically examined
by experienced mass
spectrometrists

Expanded for Quality

75% increase in coverage from
high quality sources
(129,136 spectra)

107,886	compounds
107,829	chemical structures
21,250	Replicate Spectra
13,205	Compounds with Replicate Spectra
93	Average Peaks/Spectrum
78	Median Peaks/Spectrum

Available with the enhanced, full-featured
NIST MS Search Program for Windows

with integrated tools for:

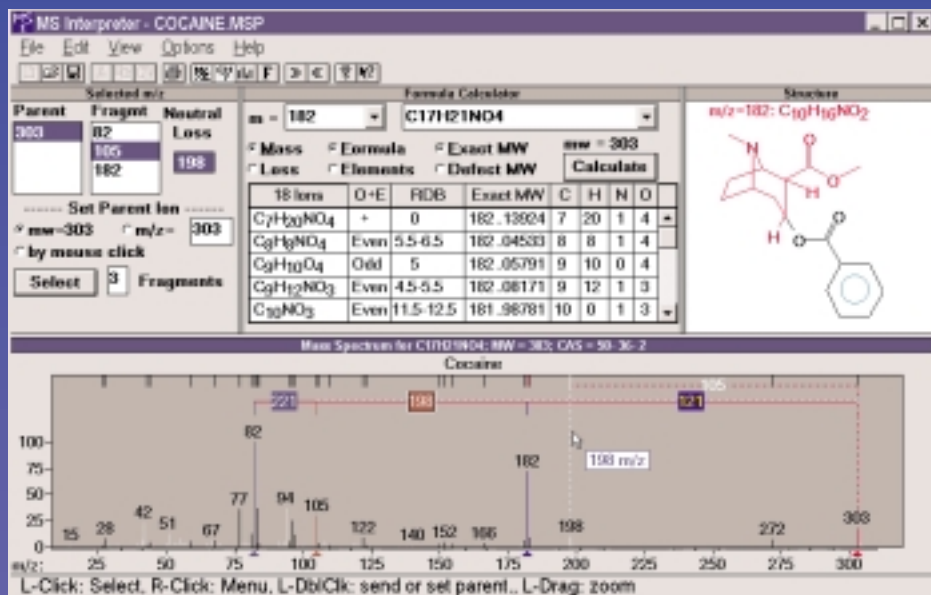
*GC/MS Deconvolution MS Interpretation
Chemical Substructure Identification*



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Mass Spectrum Interpreter

Included with the NIST/EPA/NIH Mass Spectral Database *NIST 98*



An easy-to-use, multipurpose tool developed at NIST for the evaluation of mass spectra. Examine neutral losses, isotope patterns and possible chemical formulas along with computer-assisted chemical structure/spectral analysis

Spectrum-Structure Consistency

Import a structure and a mass spectrum. Each peak is marked as either consistent or inconsistent with fragmentation rules. For each "consistent" peak, the relevant associated molecular fragment is highlighted.

Neutral Loss Analysis

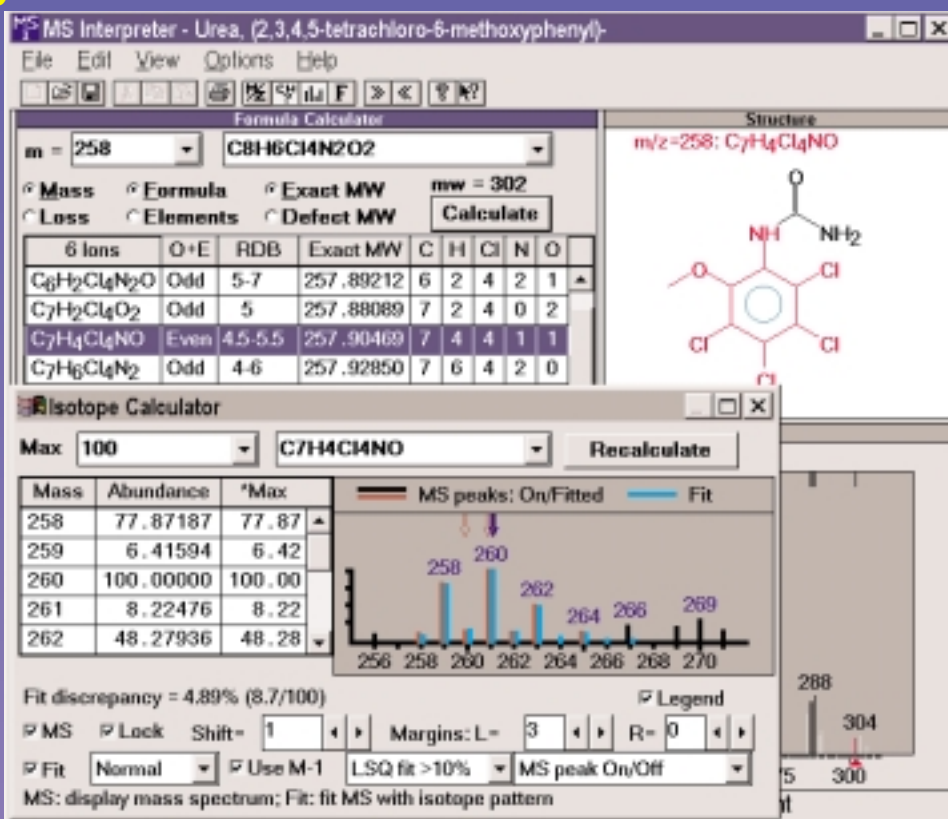
Examine fragmentation starting from the molecular ion or any secondary ion.

Isotopic Cluster Analysis

Compare proposed isotopic compositions with experiment (includes all elements).

Chemical Formula for Each Peak

Rapidly find possible elemental formulas for any peak or neutral loss in a spectrum.

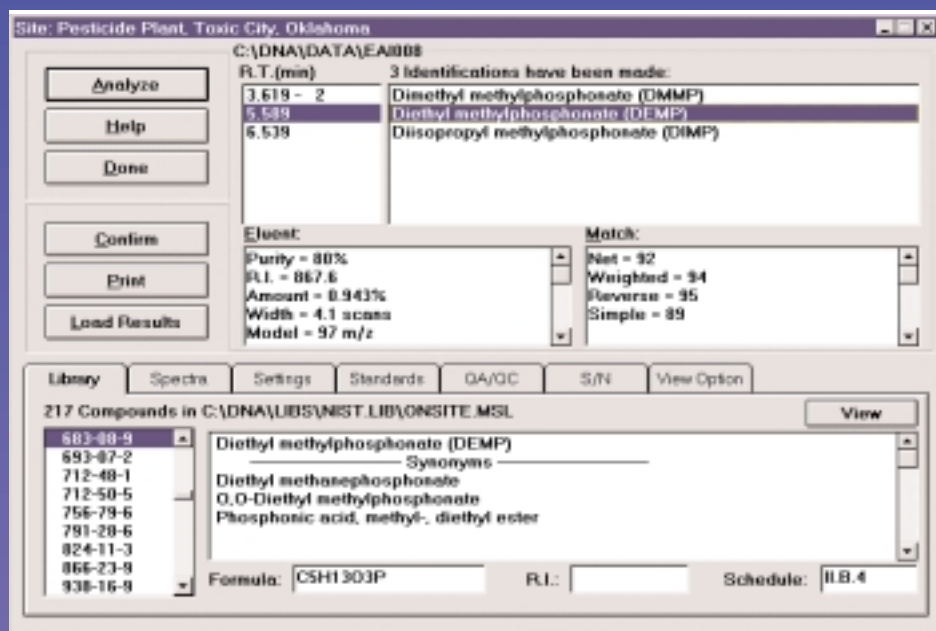


Announcing

An Automated MS Deconvolution and Identification System (AMDIS)

Included with the NIST/EPA/NIH Mass Spectral Library NIST 98

This program extracts the spectrum of each component in a mixture analyzed by GC/MS or LC/MS and identifies target compounds. With the support of the Defense Special Weapons Agency (DOD), it 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 more than two years of development and very extensive testing it is now being made available to the general analytical chemistry community.

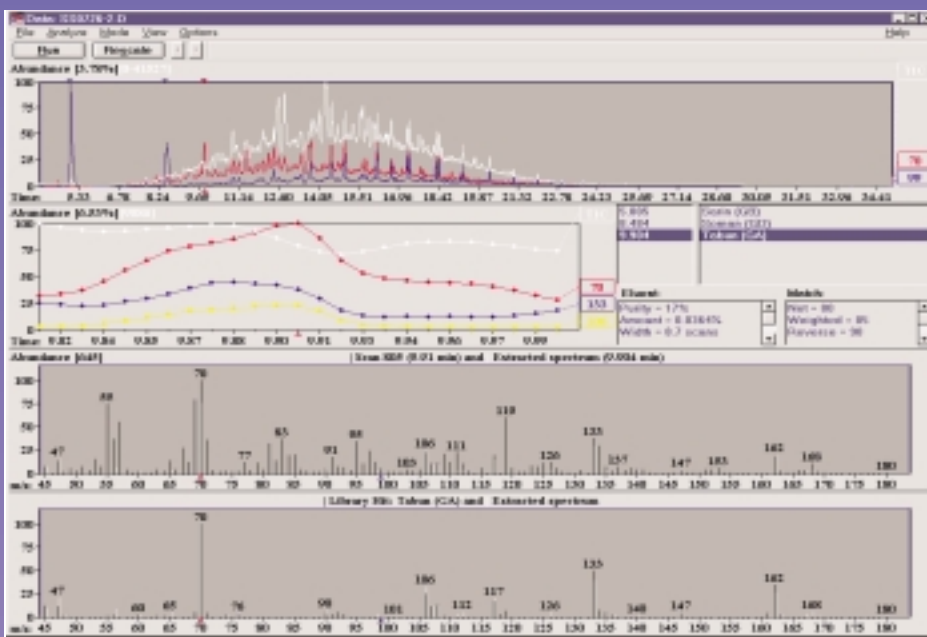


AMDIS can operate as a "black box" chemical identifier, displaying all identifications that meet a user-selectable degree of confidence.

Identification can be aided by internal standards and retention times. A performance log can be automatically maintained.

Specialty libraries derived from the NIST/NIH/EPA Database are available and custom libraries can be built directly from analyzed data files or from spectra in the NIST/EPH/NIH Database.

AMDIS can also serve as a pre-processing tool for GC/MS or LC/MS data, automatically reconstructing all original component spectra down to the limits of identification for arbitrarily complex matrices. It permits traditional library searching for any selected component. A flexible interface is provided to assist in the analysis of the most challenging matrices.



The Data

Evaluation

NIST 98 is a fully evaluated collection of electron-ionization mass spectra. It is the product of a ten-year effort by a team of experienced mass spectrometrists in which each spectrum was examined for correctness. This has led to thousands of selections, deletions and modifications to produce an optimal reference library for compound identification by spectrum matching and library searching. All decisions required agreement by two evaluators, as described in presentations at major conferences.

Expansion

A 75% increase in coverage was accomplished primarily by the addition of complete, high-quality spectra either measured specifically for the library or taken from major practical collections, including:

- Chemical Concepts including Prof. Henneberg's industrial chemicals collection
- Georgia and Virginia Crime Laboratories
- TNO Flavors and Fragrances
- AAFS Toxicology Section, Drug Library
- Association of Official Racing Chemists
- St. Louis University Urinary Acids
- VERIFIN & CBDCOM Chemical Weapons

The Software

Library Searching

Identify unknown compounds and substructures using fully documented and optimized procedures, or search by a wide range of compound and spectral properties.

Library Building

Maintain your own libraries, add your own chemical structures and search using the same optimized procedures developed for NIST 98

Flexible User Interface

Set up seven independently configured windows to examine search results and match your needs. Includes flexible printing options.

Use With Your Instrument Data Systems

Direct transfer between a number of commercial data systems and the NIST Search Program is available.

An updated version of the widely used, full-featured database software designed for identifying compounds from their mass spectra and for exploring mass spectral libraries. New tools for deconvoluting gas chromatograms and interpreting spectra are included.

