

## FEATURES

### NIST 98 and AMDIS by David Sparkman . . . . . 4

David presents us with a small teaser of tricks, techniques, and bells & whistles to be found in the NIST 98 Database and AMDIS software. David and Jane Klassen will be giving a SIS short course at ASMS.

### Advanced TOF Detector . . . . . 2

A new optically coupled detector introduced at Pittcon'99 by Galileo. S.I.S. will be the exclusive US source of this detector for the end-user market.

### Chemical Inventory/Sample Tracking . . . . . 6

Two products for Sample Tracking and Chemical Inventory satisfy a wide range of needs.

## NEW AT SIS

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### AMDIS Version 2.0 and NIST class at ASMS . . . . . 3

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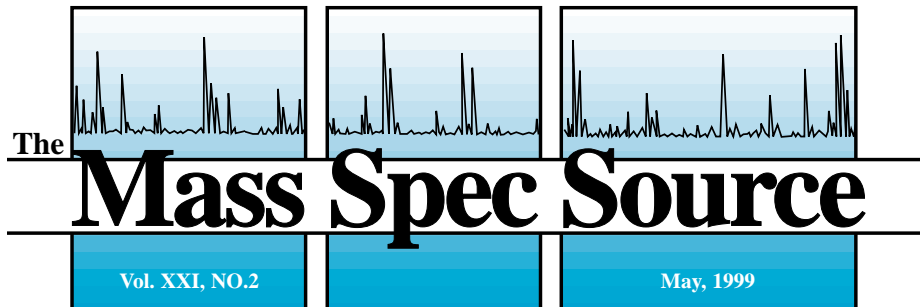
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For Mass Spectrometry and Chromatography

## ASMS Here We Come!

Join S.I.S. in our hospitality suite at ASMS for our **8th annual Ice Cream social** and view live demos of NIST 98 and SIMION 7.0 for Windows.

### SIMION 7.0 for Windows

There will be several presentations about SIMION 7.0 at ASMS. David Dahl will be giving a talk and we will present an application poster. We will also be giving demos of the SIMION 7.0 beta in our Hospitality Suite. (Ice Cream and SIMION make a great combination.) Since the news about SIMION 7.0 leaked out so early we are offering special upgrades to those who buy SIMION 6.0 now.

### NIST 98/AMDIS

Once beta testing is completed, current AMDIS users will be able to download the version 2.0 upgrade from the SIS web site. David Sparkman and Steven Stein have asked SIS to sponsor a one day class on NIST98 and AMDIS on the Sunday before ASMS. See the ad below for more details.



### NIST98 and AMDIS Course at ASMS

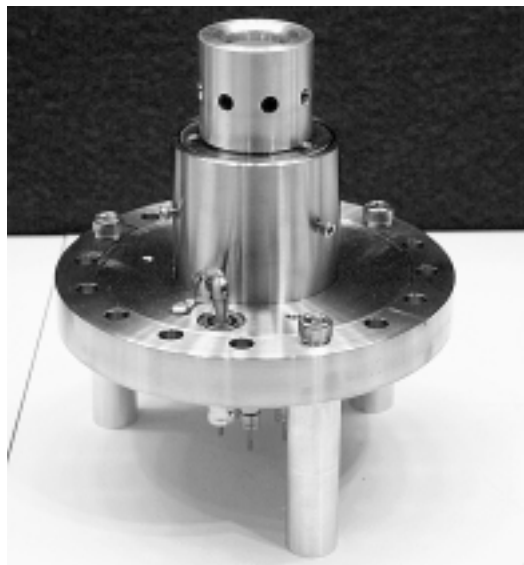
Scientific Instrument Services will sponsor a course on the NIST 98 and AMDIS Software on Sunday June 13th. 8:30 A.M.- 4:30 P.M.  
See our web site for details

### SIS Posters and Presentations at ASMS 1999

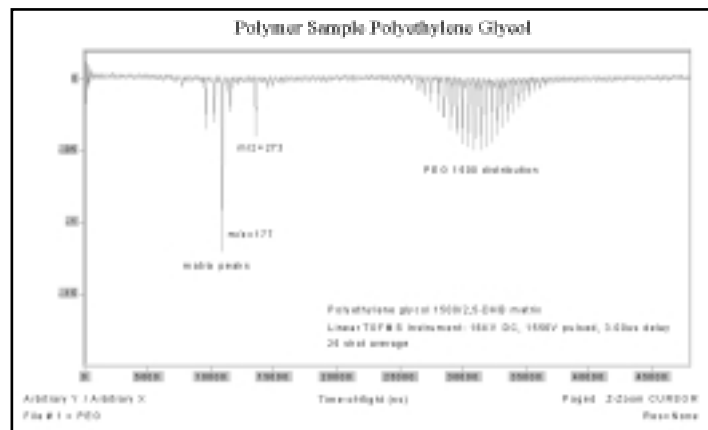
1. SIMION Version 7.0 By David Dahl (Idaho National Engineering Laboratory) Oral #287
2. High Mass Sensitivity Enhancement for Microchannel Plate Detectors By B.Laprade, H.C. Boyer; G. Grubner, N. White (of Galileo Corp.) and K. Owens (Drexel University) Poster #2067.
3. Simulation of Ion Mobility Spectroscopy Using **SIMION 7.0** By Steve Colby.
4. EPA Method TD1/TD2 Air Analyses by Automated Short Path Thermal Desorption - Gas Chromatograph - Mass Spectrometry. By Vinod Das.

## New TOF Detector

Galileo presented a new optically coupled detector at PittCon99. Scientific Instrument Services will be the exclusive US

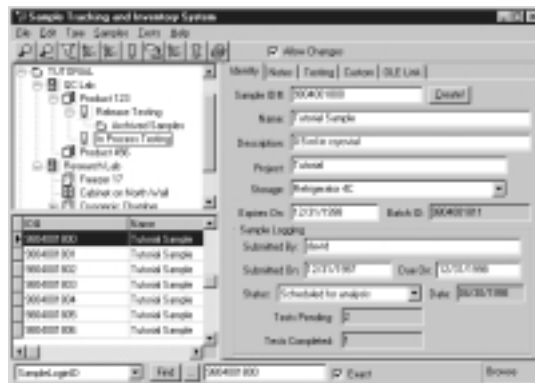


source of this detector for the end-user market. This product represents a dramatic improvement in detection of high mass ions in TOF. The figure below shows the mass spectrum of a polymer recorded with the new detector. The mass envelope observed for the polymer is almost an exact match of the theoretical Gaussian profile. For more information visit the SIS web site at [www.sisweb.com](http://www.sisweb.com).



## The Sample Tracking and Inventory System (STIS)

This software provides a host of features for tracking the flow of samples through a facility, or just keeping track of where they are stored.



STIS provides customizable fields with drop down lists for sample name, description, project and storage requirements. It provides fields for expiration and sample submission information, sample status, a large number of user-customizable fields, and an unlimited length notes field. In addition to these fields, STIS supports OLE linking for storage of other relevant information on a per-sample basis. A demo is available on the SIS Giant Demo Disk. See our web site for details.

## HP Dealership

We are proud to announce that S.I.S. now has the "Perfect Fit" for your HP GC/LC and MS system. We are now able to offer our US customers the complete line of HP parts and supplies. In order to celebrate our new Hewlett-Packard Parts and Supplies Dealership SIS will be offering a very **special discount on HP columns** this summer. SIS is one of only a few companies authorized to resell HP chromatography and mass spectrometry parts. We have available a HP catalog on CD-ROM and many items will be available in our next catalog. See the ad on page 3 for further details.

### Terms and Conditions

Scientific Instrument Services (S.I.S.) continues to supply "The Mass Spec Source" newsletter as a service to our customers. Printed four times a year, it includes articles and notes on new products and procedures of interest to mass spec and GC users. Papers from all fields of scientific inquiry in which mass spectrometry and gas chromatography can play a role will be considered and subject to review. However, S.I.S. reserves the right to reject any article that is in direct competition with S.I.S. products.

### Articles and Application Notes

Editorials and reviews on new instrumentation and techniques for GC/MS will be considered for publication. These articles may be any length and our Graphics Department will aid you in any way you may need.

### Mass Spec Tips

Any new ideas or tips that could benefit other mass spectroscopists can be submitted for inclusion in this section.

### For More Information

Anyone interested in writing in any of the areas above should contact the editor of the Mass Spec Source, at (908) 788-5550. We are always trying to improve this newsletter, if you have any suggestions please give us a call. Thanks for your continued support.

### Warranty

S.I.S. does not warranty that the items described herein are usable or fit for a particular purpose. Our company makes no representation as to condition or character of the merchandise. S.I.S. will not be responsible for consequential or special damages.

## "The Mass Spec Source"

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 Production



**Scientific Instrument Services, Inc.**

1027 Old York Road  
 Ringoes, NJ 08551-1039

Phone: 908-788-5550

FAX: 908-806-6631

Web address: <http://www.sisweb.com>

E-mail: <http://www.sisweb.com/contact>

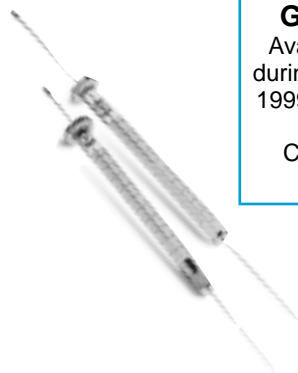
# S.I.S. Is Now An Authorized Distributor of HP Consumables and Accessories



## Limited Time Special 10% discount on HP GC & LC columns!

Available on orders placed during June, July, and August 1999. Maximum 10 columns per order.

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(908) 788-5550



Scientific Instrument Services is now able to offer the full line of Hewlett-Packard products. These include products for:

- General Chromatography
- GC and GC/MS
- LC and LC/MS
- CE and CE/MS
- ICP-MS
- UV-Vis
- Standards
- and Many More



# NIST 98

## 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*

## Expanded for Quality

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

107,886 Compounds

107,829 Chemical Structures

21,250 Replicated Spectra

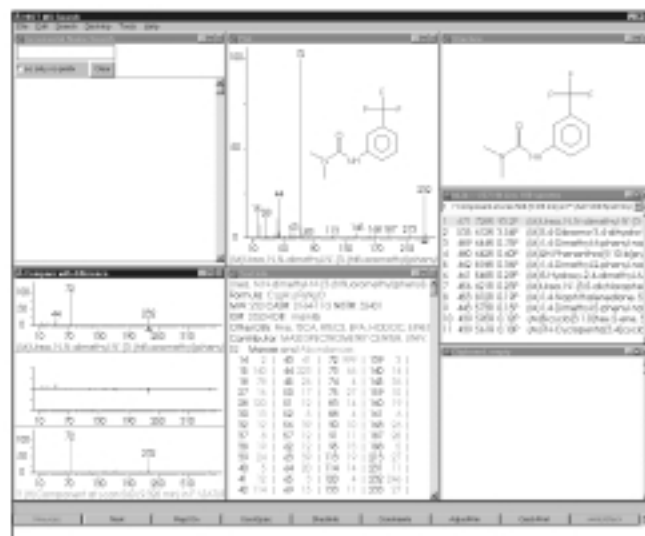
13,205 Compounds with Replicated Spectra

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



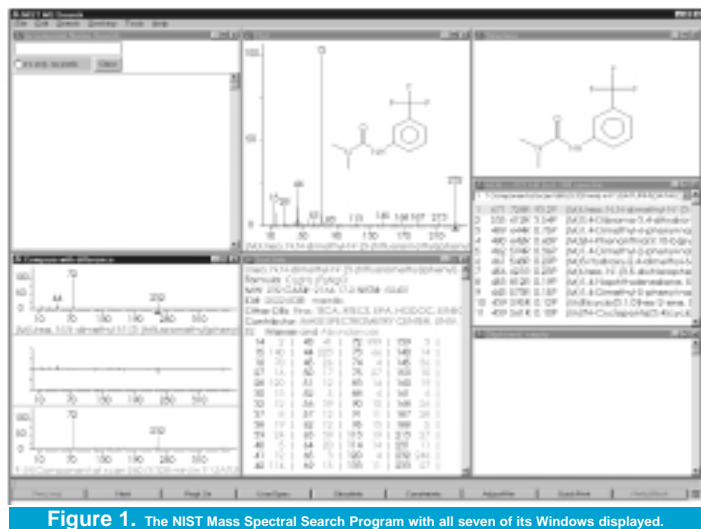
## **NIST98 and AMDIS Course at ASMS**

Scientific Instrument Services will sponsor a course on the NIST 98 and AMDIS Software on Sunday June 13th. 8:30 A.M.- 4:30 P.M.

See our web site for details

## 1998 Version of the NIST/EPA/NIH Mass Spectral Library-NIST98 *Expanded for Quality, Evaluated for Quality*

by O. David Sparkman



**Figure 1.** The NIST Mass Spectral Search Program with all seven of its Windows displayed.

### Added Features for Quality

Prior to 1998, it had been six years since NIST released its last version of the NIST/EPA/NIH Mass Spectral Library. During that period, NIST has completed a ten-year project to completely evaluate the Library. As this process progressed, NIST was able to generate a number of spectra and acquire several important collections of quality spectra. This has allowed the Library to increase in size to 129,136 spectra of 107,886 compounds. This is a 75% increase in coverage. All but 57 of the compounds have an associated structure.

In an effort to develop the Library that has been optimized for the identification of unknown compounds through their mass spectra, NIST undertook a program, using experienced mass spectrometrists, where complete-as-possible spectra were evaluated for the presence or absence of peaks based on the structure, empirical formula, and molecular weight of a compound. In the event that anomalies were found, decisions as to what should be done with a spectrum (delete from the Library, remeasure (always, where possible), or remove contaminant peaks) were reached and agreed to by two of these mass spectrometrists. This process has led to thousands of selections, deletions, and modifications to produce this optimal Library. The process of the development of the Library has been described in numerous presentations at the American Society for Mass Spectrometry meetings over the past few years.<sup>1,2,3</sup>

This new evaluated Mass Spectral Database is the NIST98 Mass Spectral Library. It is distributed along with the NIST Mass Spectral Search Program for Windows. This allows the use of either the search routines from within the mass spectral software of many manufacturers or the NIST MS Search Program itself. The NIST MS Search Program has been described in numerous publications.<sup>4,5,6</sup>

In addition to the NIST98 Database, users can also build their own libraries and have structures associated with the spectra. The Wiley 6 Registry of Mass Spectral Data is now available in the NIST format.

The NIST98 MS Search Program allows for many different Desktop configurations to be set by the user for displaying the results of the many different ways to search the NIST98 Library. Not only can unknown spectra be searched against this evaluated Database, but the Database can also be searched using incremental names of synonyms of compounds, by Chemical Abstract Services (CAS) registry numbers, empirical formula, molecular weight, and the identification number given in the Library. In addition, the Database can be searched based on data input as to the m/z value, relative or absolute intensity or type (normal, neutral loss, intensity rank in the spectrum, or whether or not it represents the maximum m/z in the spectrum) of peak. Molecular weight, unknown spectra, and peak searches can be constrained as to what elements are present as well as how many or a range of the atoms of each element can be present in a retrieved spectrum. Unknown spectra and peak searches can be constrained as to an allowable molecular weight range. Searches can also be constrained to retrieve only spectra of those compounds that are also listed in other specified databases such as those maintained by the EPA or NIH.

One of the new features in the NIST MS Search Program, V 1.6, is the ability to include user generated structures in the form of MOL files in User libraries. This feature has been a part of the HP ChemStation, but it has now been improved so that implicit hydrogens associated with functional groups are displayed.

### New Features in the NIST MS Search Program

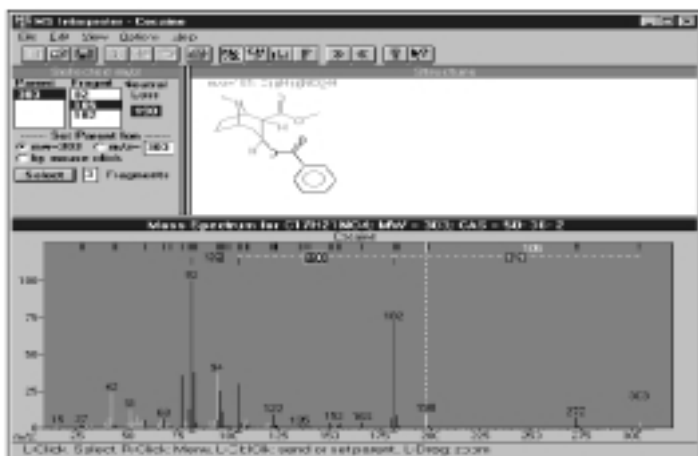
Two new features of the NIST MS Search Program are AMDIS (Automated Mass Spectral Deconvolution and Identification System) and a very unique routine that will aid in spectral evaluation and interpretation - MS Interpreter.

AMDIS will read and display GC- and LC-MSD data files from most popular instrument data systems. The files are evaluated on the basis of spectral uniqueness. Unique spectra (with contaminating peaks eliminated -deconvoluted spectra) are compared against target libraries or are sent to the NIST MS Search Program for identification. AMDIS is provided with individual target libraries (all derived from the NIST98 Library) for use with environmental, drugs of abuse, toxicological, and flavor/fragrance applications. The libraries can be expanded, and User libraries can be built from chromatographic/mass spectral data or additional spectra from the NIST98 Library or other libraries in the NIST MS Search Program format. Additional information on AMDIS will appear in a future applications note in this newsletter.

Just one of the many features of MS Interpreter is that it provides an enhancement of the popular ISOFORM utility included with previous versions of the NIST MS Search Program. This is used to calculate and display (graphical and numerically) isotopic patterns based on inputted formulas and to produce formulas for neutral fragments and ions based on molecular formula, elemental constraints, and/or m/z values of ions and neutrals.

In addition to all the functions of ISOFORM, MS Interpreter allows for a graphical comparison of observed and theoretical isotopic patterns, the ability to use a graphic tool to determine and display the m/z difference between a designated precursor peak and another peak, and, based on a simple single-bond cleavage presumption, the display of the portion of a molecular structure represented by individual peaks in the mass spectrum. This feature is a result of Robert Mistrik's Cluster Analysis research reported at the 1997 Palm Springs ASMS meeting. This powerful utility just adds to the ability of using the NIST MS Search Program and the NIST98 Library in the identification of compounds whose spectra are not in the Database.

The NIST MS Search Program, V 1.6, is still provided with three search algorithms (the Identity Search for spectra of compounds whose spectrum is probably in the Library, and the Similarity and Neutral Loss Searches for spectra of compounds whose spectrum is probably not in the Library) that has made it such a widely used utility in mass spectrometry laboratories. This later feature, combined with Substructure Identification, is one of the factors that is being extensively used in the evaluation of APCI and ESI LC/MS spectra obtained by in-source collisionally activated dissociation (CAD) or MS/MS.



**Figure 2.** MS Interpreter - a tool within the NIST MS Search Program that allows for a number of different functions including the ability to calculate the distance between peaks and determine if mass spectral peaks are logical based on an associated structure.

### Important Collections Now Included in the NIST/EPA/NIH Mass Spectral Library

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

### What IS Quality?

At issue, under many circumstances, is what is meant by the word "quality". This word has often been used as a size-comparative measure when it comes to mass spectral libraries. In the past, the basis for judgment has been the number of spectra; however, this has changed with the NIST98 Library. The NIST98 Library's total number of peaks/average number of peaks/median number of peaks values (10,033,398/93/78) are far greater than those of the only other large spectrum number/mass spectral library (the Wiley Registry of Mass Spectral Data n 8,087,622/35/10)6.

As can be easily imagined, with the numbers of spectra in the tens of thousands, the possibility of duplicating a given spectrum is very possible. This has been a problem with all previous mass spectral libraries. The only way to assure that this is not a factor is to have some unique identifier associated with

each unique spectrum. This is best accomplished by the use of a CAS registry number or a structure. The NIST98 Library has a larger percentage of spectra with a unique identifier than any other mass spectral library that has been distributed. Of all the compounds in the NIST98 Library, 99.95% have an associated structure. These unique structures were compared using one of the many in-house-developed software programs utilized by NIST to assure the highest quality. Remember, there is a difference between replicate spectra (multiple spectra of the same compound from different sources) and duplicate spectra (the same spectrum presence in the library with different index numbers).

### Summary

In combination, the NIST98 Library and the NIST MS Search Program represent one of the most powerful tools for the mass spectrometrists. As with any power tool, there are a lot of features that require training to fully implement. Consider joining our course at ASMS this year.

### References

1. P. Ausloos, C. Clifton, S. Lias, A. Mikaya, S. Stein, D. Sparkman, D. Tchekovskoi, V. Zaikin, D. Zhu "The Critical Evaluation of a Comprehensive Mass Spectral Library", *J. Am. Soc. Mass Spectrom.* **1999**, 10, 288-299.
2. V. Zaikin, P. Ausloos, C. Clifton, S. Lias, A. Mikaya, D. Sparkman, S. Stein "The Evaluation of a Comprehensive MS Reference Library", *Proceedings of the 43rd ASMS Conference on Mass Spectrometry and Allied Topics*, Atlanta, GA, **1995**.
3. S. Stein "Estimating Probabilities of Correct Identification from Results of Mass Spectral Library Searches", *J. Am. Soc. Mass Spectrom.* **1994**, 5, 316n323.
4. S. Stein, D. Scott "Optimization and Testing of Mass Spectral Library Search Algorithms for Compound Identification", *J. Am. Soc. Mass Spectrom.* **1994**, 5, 859-866.
5. S. Stein "Chemical Substructure Identification by Mass Spectral Library Searching", *J. Am. Soc. Mass Spectrom.* **1995**, 6, 644-655.
6. These figures are based on reprint of a paper distributed by F. W. McLafferty et al. in conjunction with a Poster Presentation at the 45th ASMS meeting in Palm Springs, CA, **1997**.

Part No.	Description	Price
221010	NIST 98	\$2000.00

# Managing Chemical Inventory With CISPRO

By Brian Stafford, ChemSW

Chemicals are inventory, and like any business inventory, they have to be managed economically and wisely. You have to assure that necessary supplies are on hand, but you don't want to tie up funds by overstocking or re-ordering until the materials are actually needed. Chemicals are a special kind of inventory which requires a significant information management effort:

- Chemicals must be transported, stored, handled, and disposed of safely.
- Your employees, your customers, and your community may have the right to obtain information about chemicals used in your processes or stored on your site in case of an accident or spill, rapid access to accurate information can save lives.

Maintaining chemical inventory information is a critical business requirement for large laboratories, but it is important and required for small labs and businesses as well. Material Safety Data Sheets (MSDS) are now routinely kept in many places you would not immediately think of as chemical facilities, such as hospitals and electric power generating stations.

## Track Chemicals and Supplies

The leading software system for tracking chemicals and laboratory supplies is CISPRO™, the Chemical Inventory System Pro. Together with the separate product MSDS Digital File Cabinet (MSDS DFC)™, CISPRO offers a comprehensive, scalable, and flexible solution capable of meeting both the general and specific requirements of all organizations that maintain chemical inventories. CISPRO can also connect with ChemOffice the favorite of chemists worldwide for managing chemical structural data.

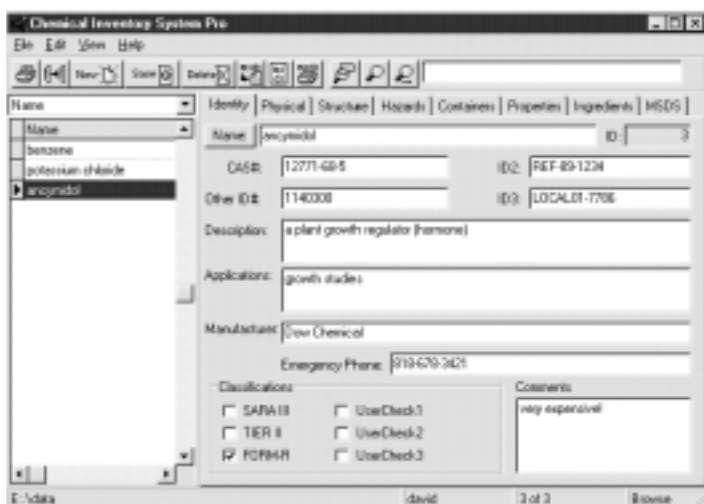


Figure 1

CISPRO works in a single-user mode or in a network environment. It stores a tremendous amount of information about each chemical, classified by the set of topic tabs shown in Figure 1. CISPRO uses a container-based tracking model, so you can manage information about multiple lots and containers of any item. Identification numbers can be linked to bar-coding systems for inventory control purposes. The Ingredients tab makes it possible to define formulations which contain multiple chemicals, and to produce scaled batch reports for material requirements applications. As a result, CISPRO is not limited to pure chemicals - it can track anything in your storeroom, laboratory, or plant.

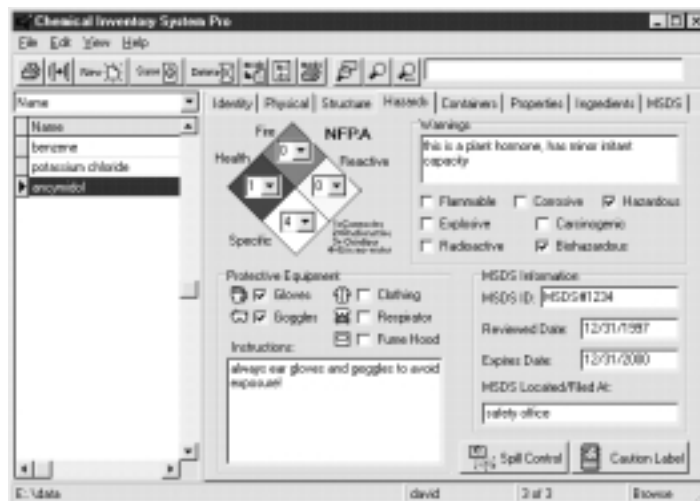


Figure 2

The Physical data tab contains a variety of information such as formula, molecular weight, physical constants, physical form, and storage compatibility. The Hazard data tab, Figure 2, conforms to the NFPA Hazard Rating System (fire, health, reactivity, and specific hazards) and also maintains a link to the Material Safety Data Sheet in the Digital Filing Cabinet (a separate SIS product).

At the most detailed level, some installations may want to monitor each addition or removal of an item or a quantity of stock. CISPRO has an optional transaction-logging system which records item, date, location, user, and reason for transfer. It can produce reports and warnings when supplies drop below a specified level, and it provides cost-accounting functions such as removal and addition costs per account or value of inventory.

## Use CISPRO with ChemOffice

While safety officers, inventory managers, and other non-technical users of CISPRO usually look up items in the system by name, CAS Registry Number, or a similar text field, chemists may want to locate items using a structure search. For example, a research chemist may have devised a brilliant new synthesis route, but to try it he'll need 500 grams of methyl 2-iodobenzoate. Is it in the building, or on the campus? If so, where? To answer these questions without any concern for ambiguities of nomenclature,

the scientist may prefer to sketch the structure and search for the compound that way.

To connect with ChemOffice, the CISPRO has added a Structure tab to display the structure. Chemical structures can be imported into CISPRO by selecting a ChemDraw file or by searching a ChemFinder database. The chemist can browse through the

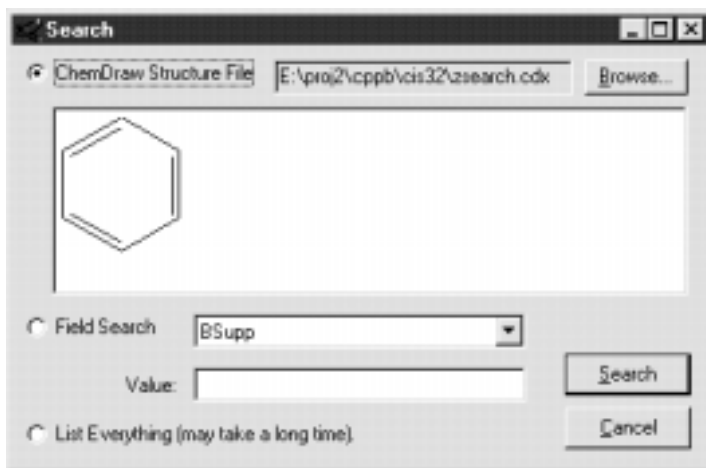


Figure 3

records in CISPRO, or ask to search by structure. CISPRO then calls on the ChemFinder component of ChemOffice to conduct the structure, substructure, or similarity search. See Figure 3. The mechanism for this link is the ChemFinder/CIS32 OLE Automation Interface, which makes different software packages under Windows work together as if they were a single program.

## Manage Safety Data

When it becomes necessary to obtain the safety information related to an inventory item, CISPRO can retrieve data stored in its own format or connect to Material Safety Data Sheets in the MSDS Digital Filing Cabinet (MSDS DFC). This application is a document imaging facility designed to store and retrieve Material Safety Data Sheets as images. Instead of wading through stacks of papers in 3-ring binders or file cabinets, you quickly locate the required MSDS stored in your computer and view it on your computer monitor.



Figure 4

Storing MSDSs in the filing cabinet means that there is a single copy maintained in one place, available throughout your network. The DFC makes it simple to replace or update a page, and even automatically generates request letters to suppliers for new copies of MSDSs.

How do you get your MSDSs into the DFC in the first place? The DFC is smart: its Document Acquisition Wizard, leads you through the entry process for a variety of sources, including scanners, FAX modems, text files, various applications, or directly from the keyboard. It even knows how to import MSDS sheets from several Internet MSDS Servers on the World Wide Web.

## CISPRO in Action

CISPRO is used in many industrial, academic, and government sites. Let's take a look at some representative examples.

At a large consumer health care manufacturing facility, CIS Pro is going into action in the QC/Analytical labs. This large plant regularly uses thousands of chemicals, and one of the first jobs CISPRO will tackle is consolidating a shelf full of MSDS sheets in 3-ring binders. The lab director notes that "The system's security measures protect read-only information like the MSDSs, but lets us allow password access to the parts we need to update." Solvent accounting is another major task. "The system will keep track of the quantities and types of solvents that people check out and give us monthly usage reports, which we can tie to re-ordering and accounting."

Lewis & Clark College in Portland, OR upgraded from a simple non-chemical database method of record-keeping to CISPRO. Gillian Gardner, Lab Director and Instructor in Chemistry, noted CISPRO's chemical intelligence puts the lab's 2,000 chemical names in the correct sequence. "We also chose CISPRO because it could track the age, grade, and source of our chemicals, link chemicals to courses, and provide with us with cumulative usage statistics," she commented. The new system will also make it easier to see when inventories fall below re-order levels. Finally, with bar-coding in place, the system will keep much more accurate accounts of removals and additions."

Together, the MSDS Digital Filing Cabinet and the Chemical Inventory System Pro make up a highly capable, flexible chemical tracking system suitable for small or large organizations. CISPRO works with ChemOffice, the favorite software of chemists for working with structures and models. CISPRO takes care of the specialized needs of chemical tracking and also makes critical information available to both local and remote users. Electronic filing of MSDS documents eliminates shelves of paper while making the stored information available to any connected computer. Lab managers, purchasing agents, safety officers, and chemists will all find that CISPRO and MSDS DFC help them spend less time tracking down information and more time making use of it.

ChemOffice, CISPRO, and MSDS Digital Filing Cabinet are separate products and must be ordered separately. Barcode systems available as separate options.

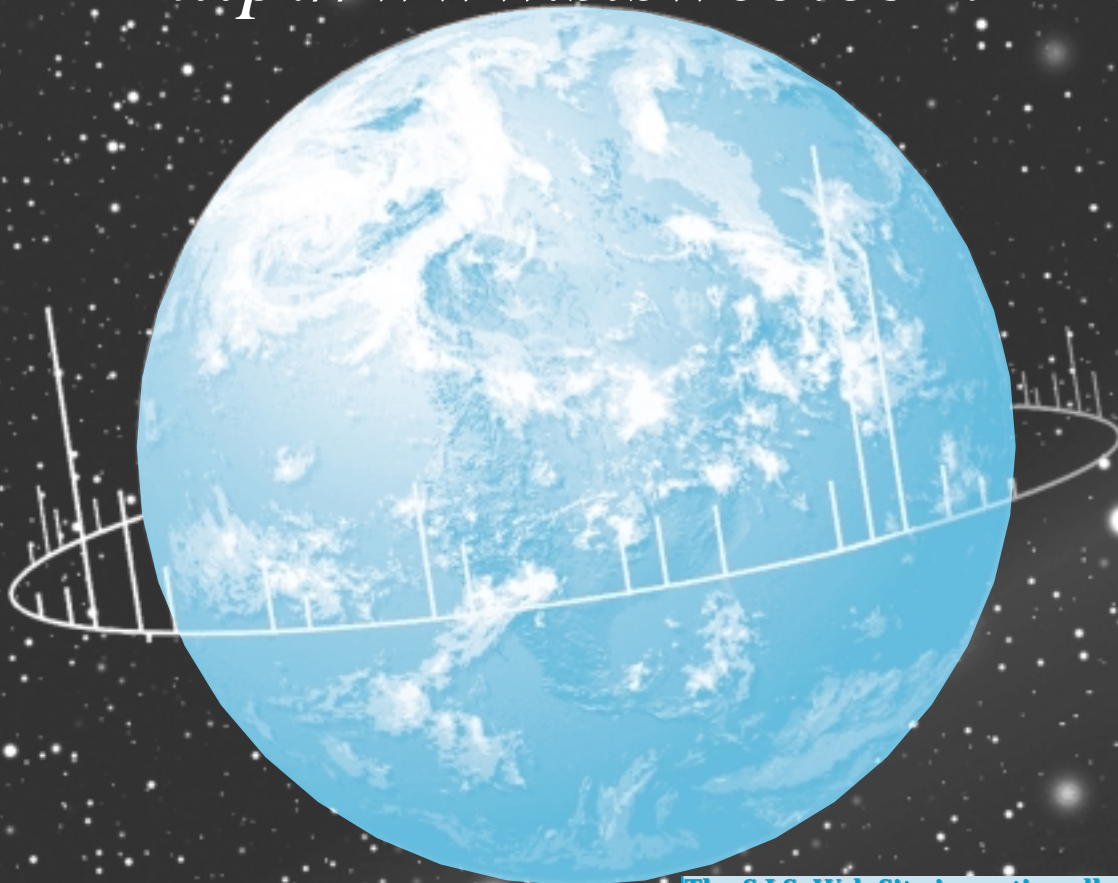
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Part No.	Description	Price
12220	CISPRO2000	\$1299.00
12195	MSDS/DFC for CISPRO	\$899.00

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*<http://www.sisweb.com>*



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New Application Notes:**

*Design, Development and Testing of a Microprocessor Controlled  
Automated Short Path Thermal Desorption Apparatus*

*Volatile Organic Compounds from Electron Beam Cured and  
Partially Electron Beam Cured Packaging Using Automated Short  
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*Rapid Bacterial Chemotaxonomy by Direct Probe/MSD*

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