NIST Mass Spectral Libraries in Forensic Trace Analysis

Trace Evidence Data Workshop
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MS Applied to Forensic Trace Analysis

… a (very) partial list

- Toxicology/cause of death
  - urine, blood
  - hair, saliva, sweat
- Profiling
  - determination of sample origin
- Explosive/gun shot residues
  - Linking residues to people
- Arson investigation
  - Determination of accelerants
- Paints/inks/dyes/colorants
- Pharmaceutical adulterants
  - Especially in the developing world
- …

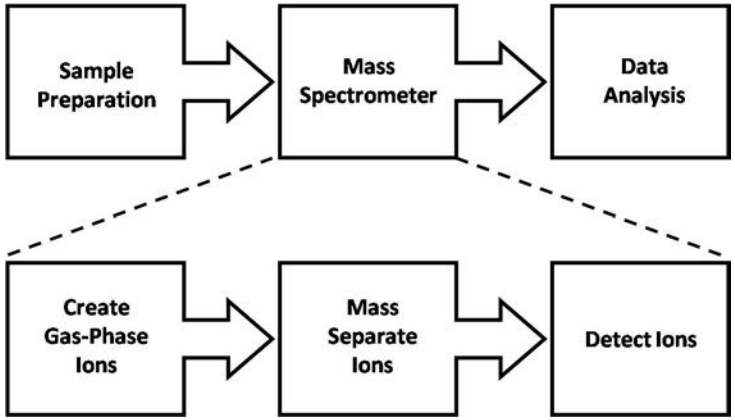
a NIST MSDC mass spectrometry lab

Why Mass Spectrometry?

Mass spectrometry is developing rapidly in the areas of sensitivity, specificity, and analytical throughput

- **Handling of small volumes**
- **Clean up of complex samples**
  - **solid phase extraction**

- **Development of new software tools**
- **Sophisticated new algorithms**



- **New ionization methods**
  - **DART**
- **Greater efficiency in ionization**

- **Increased mass resolution**
- **Increased ion throughput**

- **Improved signal to noise**
- **New signal processing approaches**

The NIST Mass Spectrometry Data Center rests on a central tenet—

Libraries are a necessity in identifying compounds from mass spectra

- Why?
- There is no comprehensive theory accurate enough to predict mass spectra for the purpose of compound identification
    - Although theory is useful for interpretation
- Consequently, library creation by systematic, comprehensive measurement has a long history in mass spectrometry…

… particularly at the National Bureau of Standards

- Brewer & Dibeler, *Journal of Research of the National Bureau of Standards*, 1945
- *"The ratios in which the fragments occur are the same over a wide pressure range for each molecular species but are never the same for different species"*

U. S. Department of Commerce National Bureau of Standards

RESEARCH PAPER RP1664

Part of Journal of Research of the National Bureau of Standards, Volume 35, August 1945

MASS SPECTROMETRIC ANALYSES OF HYDROCARBON AND GAS MIXTURES[1]

By A. Keith Brewer and Vernon H. Dibeler

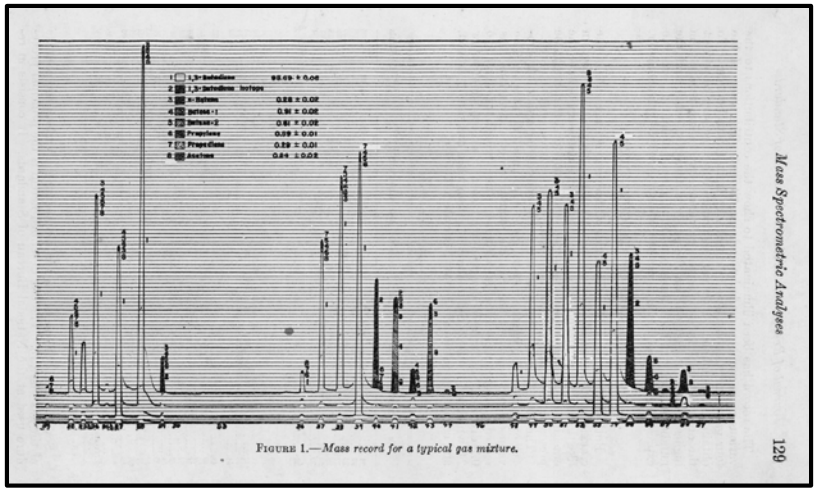
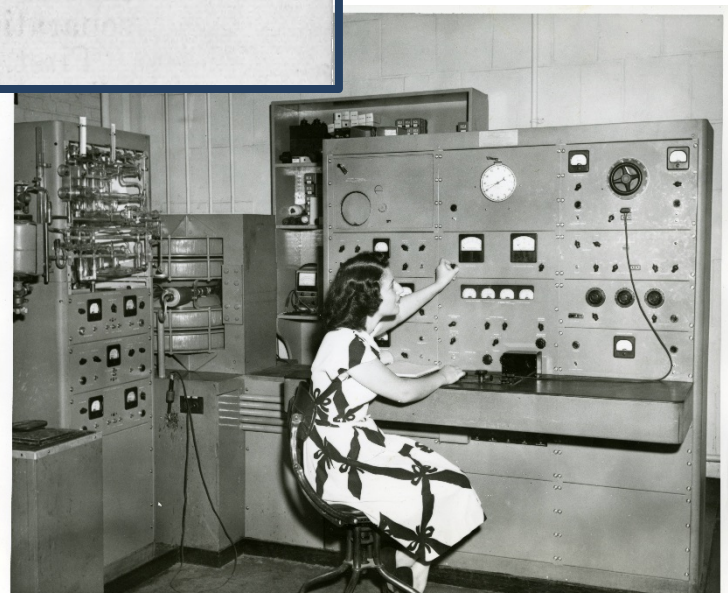


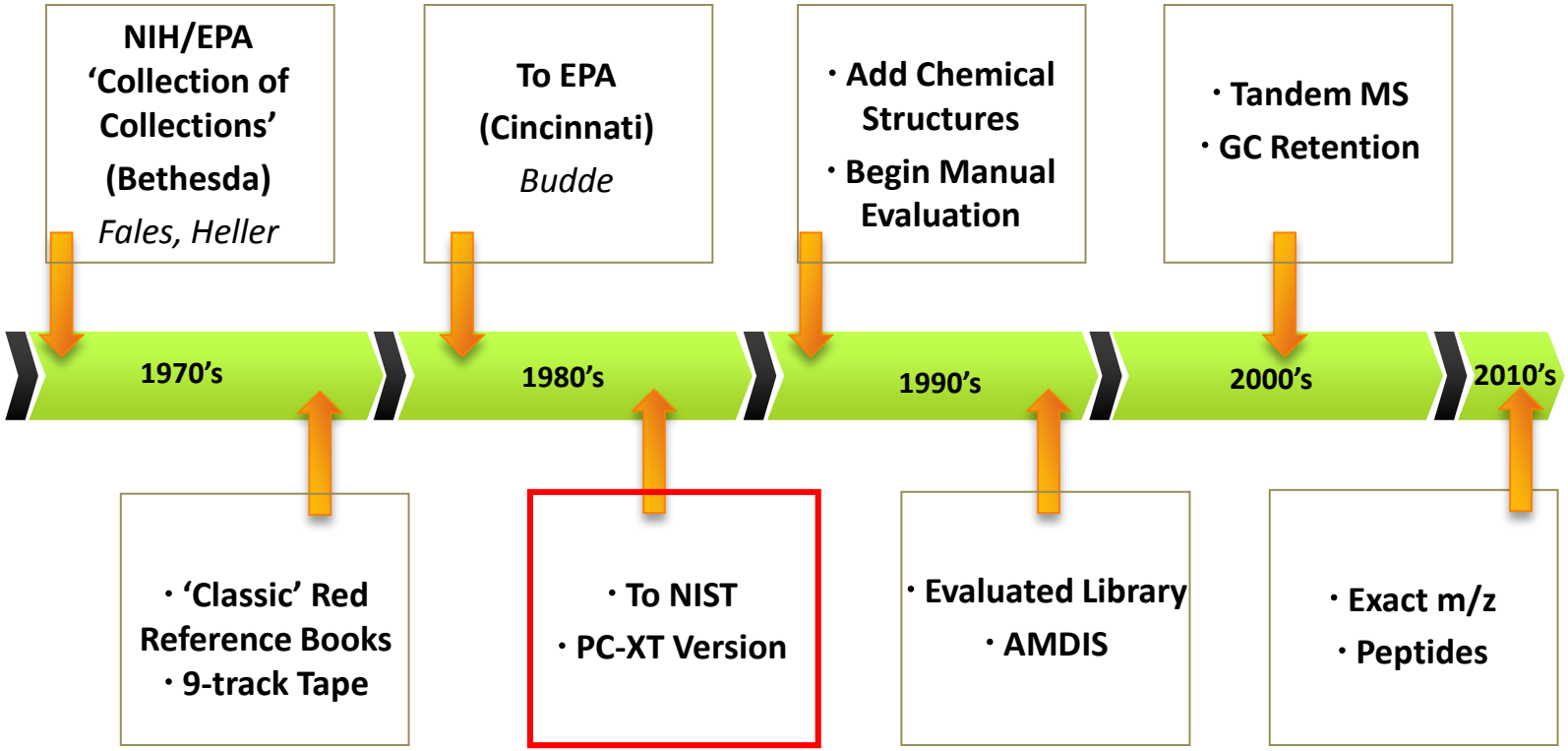
Figure 1.—*Mass record for a typical gas mixture.*

Mass Spectrometric Analyses 129

NIST Archives photo dated Sept. 29, 1948



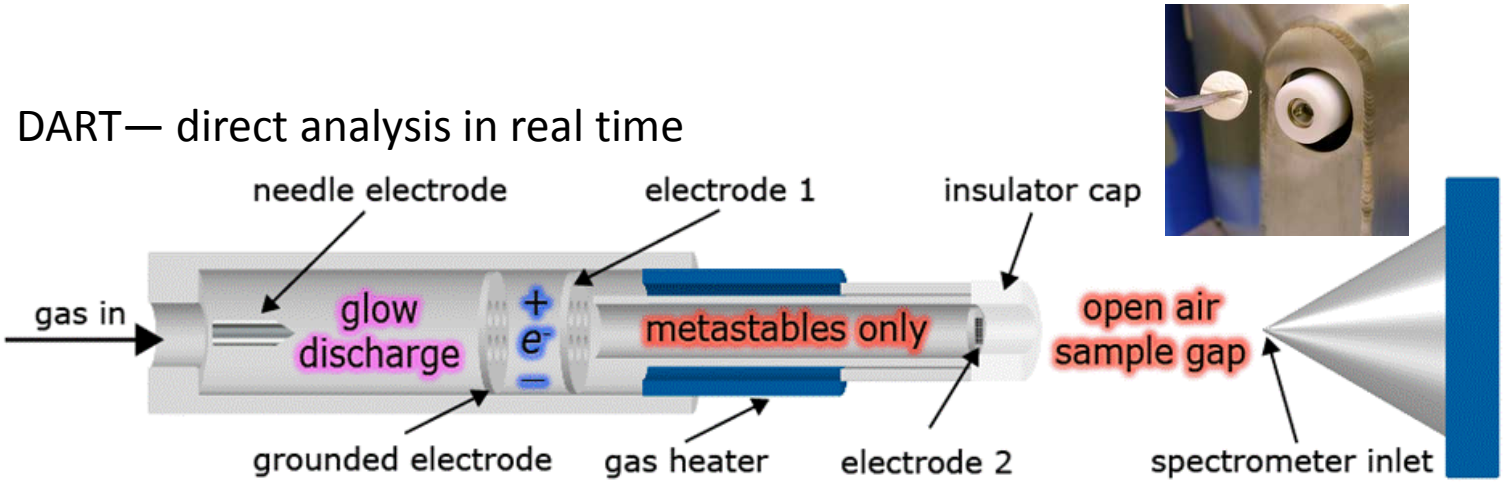
Evolution of the NIST MS Library



NIST Mass Spectral Libraries in Trace Analysis

- NIST/EPA/NIH Mass Spectral Database
  - Electron-impact ionization mass spectra typical of GC-MS analysis
- NIST Tandem MS Database
  - Electrospray ionization mass spectra typical of LC-MS analysis
- DART Forensics Library
  - For analysis directly from surfaces
  - An example of a 'targeted' library

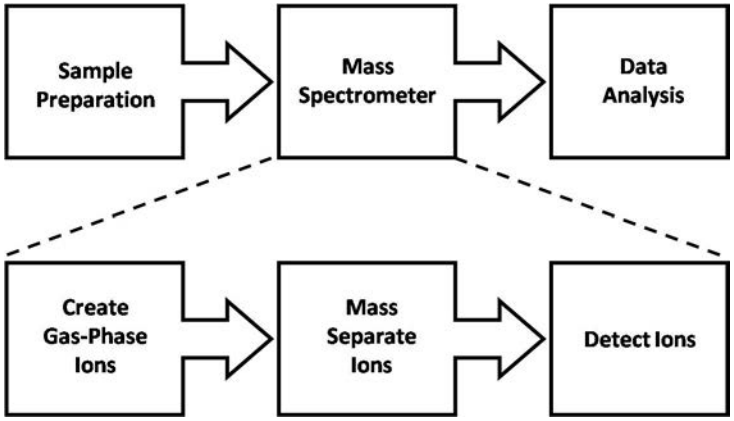
DART— direct analysis in real time



NIST MSDC Software Tools

- Handling of small volumes
- Clean up of complex samples
  - solid phase extraction

- Development of new software tools
- Testing new algorithms



- New ionization methods
  - DART
- Greater efficiency in ionization

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- Increased ion throughput

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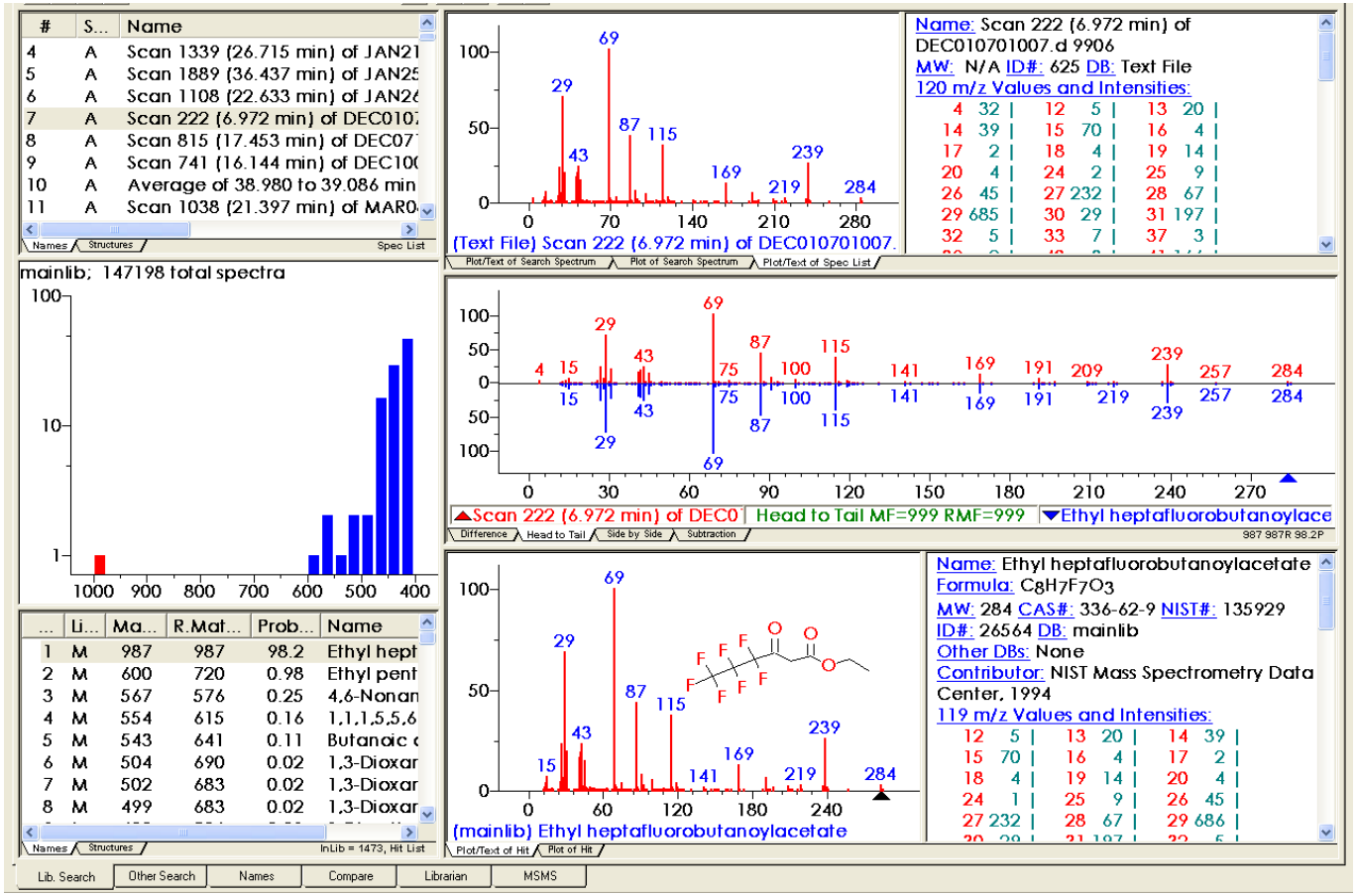
NIST GC-MS Library Search

Search List

Score Histogram

Hit List



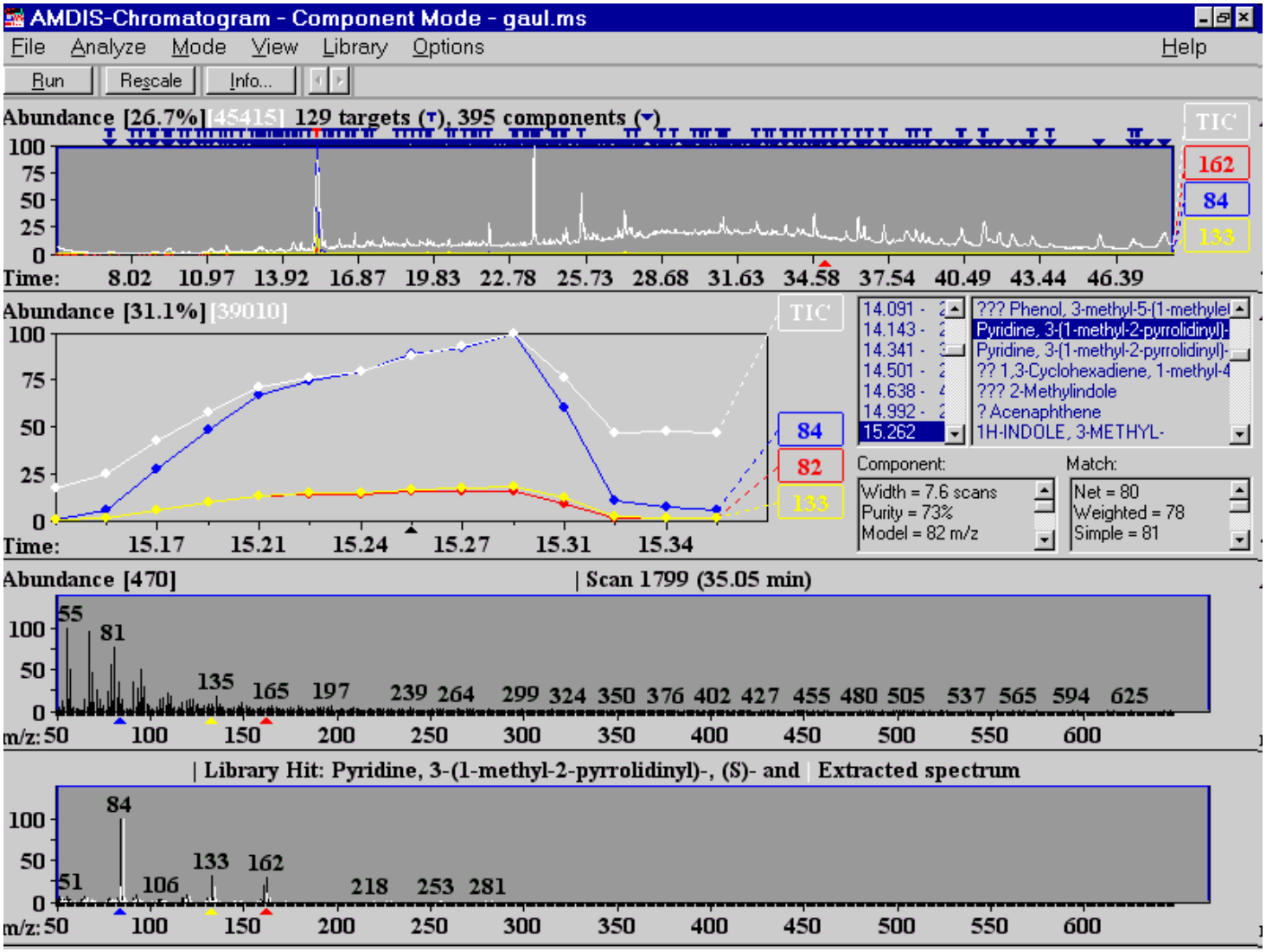
Query Spectrum

Compare Spectra

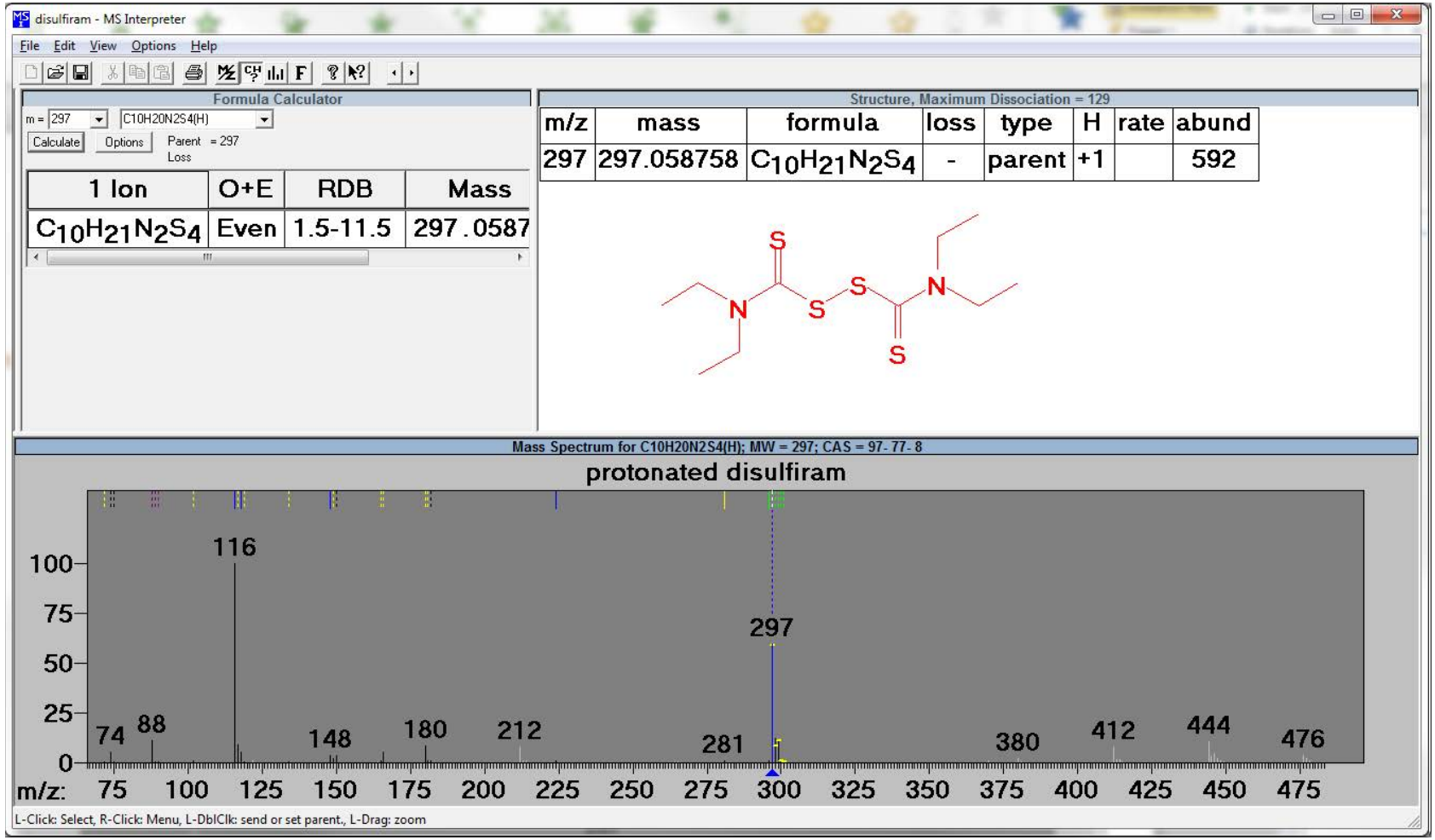
Library Spectrum

AMDIS

Automated Mass Spectral Deconvolution and Identification System



NIST MS Interpreter



What does the NIST MSDC need from the forensics community?

- What are the emerging trends that you are seeing in your labs?
- What compounds do they involve?
- How may NIST obtain certified samples?
  - purchase
  - synthesis
  - isolation from original matrix
- What can the NIST MSDC do to help build the community?
  - an interlaboratory round robin?
  - training on library searching?
  - guidance on uncertainty/false discovery rates?

MSDC staff meeting with customers at our trade show booth

Questions?