

Importance of Mass Spectral Search to Chemical Manufacturers

-ASMS 2020 Reboot Workshop #19

-Compound Identification by Mass Spectral Library Searching

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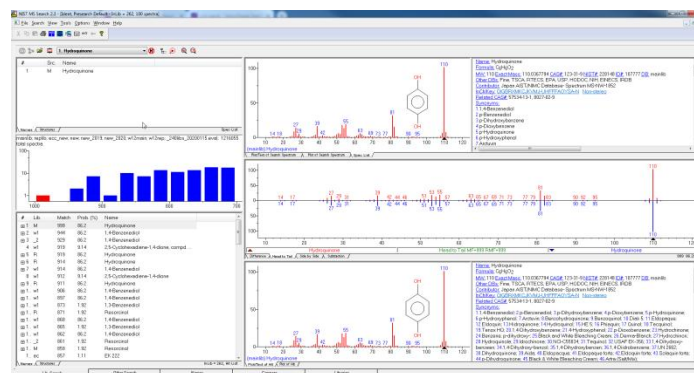
<https://littlesandsailing.wordpress.com/>

Kingsport, TN

NIST Search Used by Eastman Chemical



Eastman Chemical Co., Main Site, Kingsport, TN
50 Manufacturing Sites Worldwide, ~14,500 Employees



~50 GC/MS's, LC/MS's Networked Worldwide

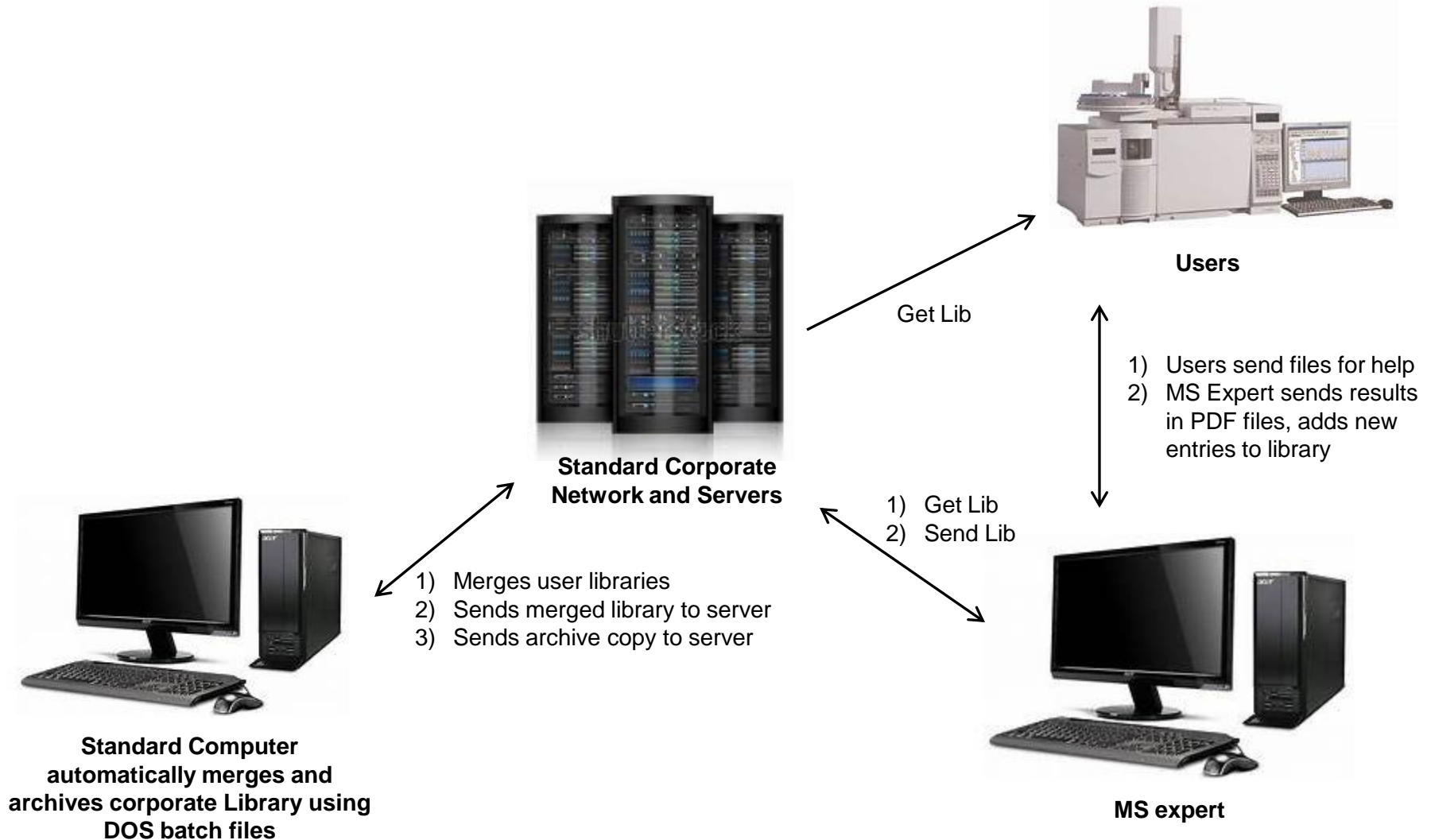
NIST Search of EI and MS/MS User Libraries
~60,000 EI and ~3,000 MS/MS spectra/structures

Process for Characterization of Samples by Mass Spectrometry at Eastman

- **Majority** of samples analyzed in remote laboratories by chemists in chromatography and synthetic laboratories
- Experience of users varies, but typically not “highly skilled” in mass spectrometry interpretation
- **If** results not found by search, files are sent to “experts” in central MS lab for identification
- “Experts” report results using annotated chromatograms (PDF files) via e-mail
- “Experts” add entries to corporate library
- **If necessary**, samples sent to central MS lab for accurate mass/chemical ionization, advanced sample preparation, *etc.*

Worldwide Network of MS Users, Instruments, and Experts

- Library updates performed **daily**
- DOS batch files utilized (e.g. "Get Lib") and standard network hardware
- Essentially **no** additional cost



Types of Components Added to Library

Anything a user would find useful, thus ***much more*** “diverse” than purchased commercial EI and MS/MS databases

Thus, users must realize Eastman database is an ***aid to identification*** and should be used accordingly.

- Most entries high quality with high confidence and exact structure
- Some entries will have “?” or “??” in front of name to show educated guess
- Many components added with reference to common names for commercial plasticizers, lubricants, surfactants, antioxidants, UV stabilizers, polyesters, *etc.*
- Many entries added with reference to plant and R&D processes with unknown structure, but do include accurate mass and confirmation of MW by CI

Information Added to Eastman Library Entry

Mass spectrum, molecular formula, molecular weight plus detailed comments, *e.g.*

- Associated Plant Material No. (PM number)
- Associated R&D common process name
- Detailed sample history
- Electronic laboratory notebook No.
- Confirmed by accurate mass, chemical ionization, NMR, etc.
- Date
- Name of submitter
- Name of expert adding entry

Importance of Library Search and Comments in User Library

Google Aerial View of Kingsport Site (~2.3 x 1.3 miles)

- MS's used in conjunction with TOC (total organic carbon) water monitors
- Quickly determine source of spills in manufacturing or breaches from water treatment plant
- Exact structure useful, but not necessary
- Comments in unknown spectrum used to determine process and pinpoint location



Summary

- Spectra imported to NIST search from all MS manufacturers data processing software
- **Both** user libraries and commercial ones used for searching
- Critical assets needed to support R&D and environmental needs in chemical industry
- NIST search can quickly search >1,100,000 EI spectra in NIST, Wiley, and user libraries
- Also, search by exact and similar structure (>1,000,000)
- User databases easily created and updated **daily**

Internet References

(Hyperlinks to Internet Resources)

1. [James Little Mass Spectral Resource Website](#)
2. [NIST Search Software Detailed Manual](#)
3. [NIST/AMDIS Program for Data Processing](#)
4. [Basic Instructions for Using AMDIS with NIST Search](#)
5. [Nightly Automatic Update of Users' Libraries](#)
6. [Using NIST Search from Instrument Manufacturers' Software](#)
7. [Chemical Ionization for MW Determination](#)
8. [Trimethylsilyl Derivatives for GC-MS](#)
9. [Methyl Ester Derivatives for GC-MS](#)
10. [SciFinder/ChemSpider and Accurate Mass LC-MS Data for Unknown ID's](#)
11. [Surfactant Identification](#)