# KnowItAll Mass Spectrometry Training

**Vendor Neutral Data Processing Solution for Spectral Analyses**

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KnowItAll™

## "Making User Library Using PubChem & MS Interpreter"

James Little
Mass Spec Interpretation Services

Handouts for Videos:
Website: Little Mass Spec and Sailing
https://littlemsandsailing.wordpress.com

**NOTE:** Series of other training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

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# Skills Needed from Previous Videos and Handouts

➢ProcessIt for obtaining an EI spectrum from a GC-MS file

➢SearchIt/MineIt for searching a mass spectrum

➢Tips for drawing structures using ChemWindow

**NOTE:** Internet links to my FREE course on using NIST MS Interpreter can be found in the associated handout for this video

# Another Useful Reference on Databases



**Quick Reference Guide**

**KnowItAll**
Analytical Edition

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**Fall 2022**
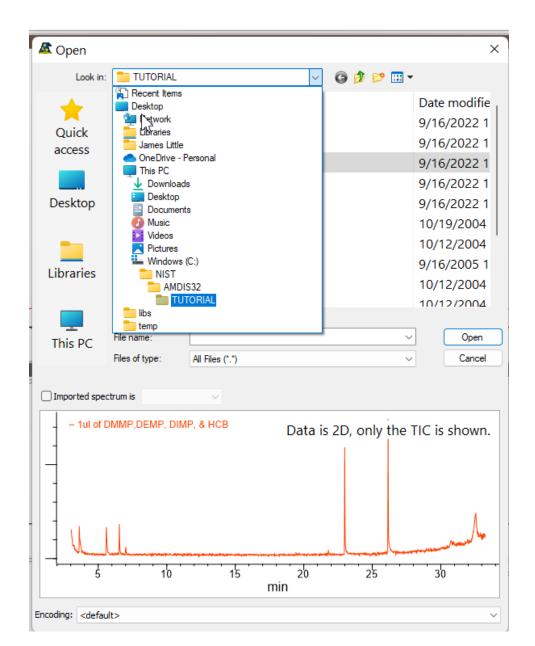
**Prepared By**
**O. David Sparkman**

**How to Use KnowItAll Mass**
**Spectrometry Applications**

***NOTE:*** Link to Quick Reference Guide found on my personal website

# File Used for Demonstration

File supplied with AMDIS NIST
Software in their Tutorial Folder

# Process for Creating User Library (Database)

➢Create a user library (database) in MineIt

➢Obtain a spectrum for first entry using ProcessIt

➢Transfer to MineIt

➢Draw a structure in ChemWindow

➢Transfer to MineIt and add to first record

➢Check quality of spectrum using NIST MS interpreter in MineIT

➢Add any fields of interest using PubChem option in MineIt

➢Add a comment field

➢Continue process to add a second record

➢Check by picking one of the entries added and search **5**

**Training for NIST MS Interpreter to Understand EI Fragmentation**

➤The use of MS Interpreter can be found in links shown below
➤Will take a little effort on user to become proficient

*Links to References (click on them)*

-*video tutorial*
-*handout for video tutorial*
-*other useful references*

# *Other* Training of Newly Released Wiley KnowItAll Mass Spec Software on My Website

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